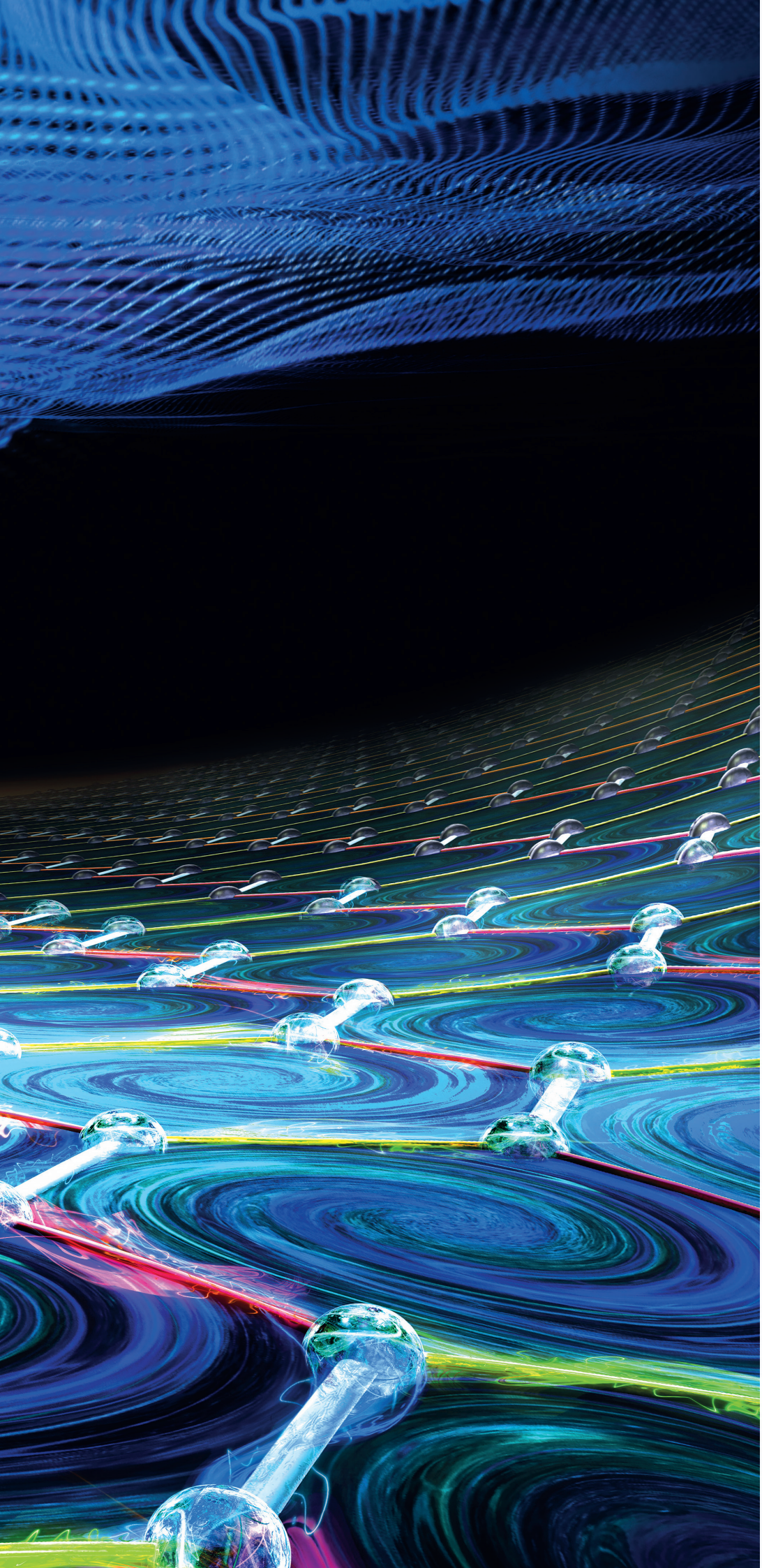

Max Planck Institute
for the Physics of
Complex Systems

Scientific Report

10/2021–12/2024

mpipks

Front cover
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Quantum vortices interact with quantum matter under
strong periodic driving.

IMPRESSUM

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Contents

Chapter 1

Scientific Work and its Organization at the Institute – an Overview

1.1 History and Development of the Institute

1992-1994 • The Max Planck Institute for the Physics of Complex Systems (mpi**pks**) was founded by the Senate of the Max Planck Society in November 1992. The concept for the institute envisaged three scientific divisions and a large Visitors Program. The mission is to contribute to the research in the field of complex systems in a globally visible way and to promote it as a subject. One of the central goals is to pass on the innovation generated in the field as quickly and efficiently as possible to the young generation of scientists at universities. Dresden was chosen as the location for the institute for its favorable scientific environment and its location near the German-Polish-Czech border triangle. In July 1993, Founding Director *Prof. P. Fulde* launched the scientific activities of the first division *Electronic Correlations* in Stuttgart. Work in Dresden started in January 1994 thanks to the TU Dresden which generously offered a temporary accommodation for the institute. The institute was officially inaugurated by *Prof. H. Zacher*, President of the Max Planck Society, on May 2nd, 1994. An administration was installed headed by *Mrs. I. Auguszt*. The Visitors Program began to operate, first guests were invited, and the first workshop took place in March 1994.

1995-1998 • In 1995, *Dr. H. Kantz* joined the institute as head of an independent Junior Research Group on *Nonlinear Time Series Analysis*. Moreover, the mpi**pks** decided to broaden its research spectrum considerably by installing temporary Junior Research Groups: The group *Pattern Formation in Reaction-Diffusion-Systems* headed by *Dr. M. Bär* started its activities in 1995, the group *Quantum Chaos and Mesoscopic Systems* headed by *Dr. K. Richter* in January 1996, and the group *Quantum Chemistry* headed by *Dr. M. Dolg* soon after. At the same time, plans for the institute's building and guest houses took shape. The architects Brenner und Partner (Stuttgart) won the competitive bidding, and construction started in September 1995. After less than two years the institute moved into the new main building and took into service the three guest houses. In the meantime, the Workshop and Visitors Program gained momentum with hundreds of scientists visiting the institute.

1999-2001 • In 1999, the *Finite Systems* division was installed under the direction of *Prof. J. M. Rost*. In the same year, *Dr. A. Buchleitner* arrived at the institute to launch the research group *Nonlinear Dynamics in Quantum Systems*. *Dr. U. Birkenheuer* succeeded *Dr. Dolg* as head of the *Quantum Chemistry* group in March 2000. To strengthen the successful work in mesoscopics, *Dr. H. Schomerus* was appointed as head of a new Junior Research Group *Waves in Complex Media and Mesoscopic Phenomena* in November 2000.

2001-2002 • In 2001, *Prof. F. Jülicher* was appointed as head of the third division *Biological Physics* establishing a bridge between physics and biology. Shortly afterwards, two research groups on *Physics of Biological and Soft Matter* headed by *Dr. R. Everaers*, and *Biological Physics of Olfaction: From Genes to Networks* headed by *Dr. M. Zapotocky* started their activities. Moreover, the division *Finite Systems* continued to broaden its research spectrum by appointing *Dr. A. Becker* as head of the new research group *Nonlinear Processes in Strong Fields*.

2003-2004 • In 2003, *Dr. S. Kümmel* set up the Emmy Noether Group *Electronic Structure of Finite Systems* at the Institute. In the following year, the mpi**pks** and the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) launched the joint research program *Physics of Biological Systems* and established its first two Junior Research Groups: *Dr. K. Kruse*, head of the group *Physics of Cell Division*, working theoretically at the mpi**pks**; *Dr. I. M. Tolić-Nørrelykke*, head of the group *Mechanics of Cell Division*, experimentally at the MPI-CBG.

2005-2006 • In 2005, *Dr. M. Hentschel* started the activities of the Emmy Noether group *Many Body Effects in Mesoscopic Systems*. *Dr. S. Grill* completed the joint research program of the mpi**pks** and the MPI-CBG by launching the Junior Research Group *Motor Systems*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* started operation and the new wing of the institute was completed providing additional office space and a new seminar room.

2007-2008 • During this period *Prof. P. Fulde* retired from his position as a director of the mpi**pks** and head of the division *Electronic Correlations*. *Prof. R. Moessner* was appointed as new director, and started to set up his division *Condensed Matter* in early 2008. Several new groups were installed: In 2007, *Dr. T. Gross* joined the mpi**pks** to head the Junior Research Group *Dynamics of Biological Networks*, and *Dr. B. Lindner* set up the activities of the research group *Stochastic Processes in Biophysics*. In the same year, *Dr. S. Skupin* started his Junior Research Group *Computational Nonlinear and Relativistic Optics*, with close links to the Helmholtz Center Dresden-Rossendorf. In 2008, the research groups *Complex Dynamics in Cold Gases* and *New States of Quantum Matter* were founded under the direction of *Dr. T. Pohl* and *Dr. A. Läuchli*, respectively.

2009-2010 • In 2009, *Dr. S. Kirchner* joined the mpi**pks** as head of the Junior Research Group *Collective Phenomena in Solid State and Materials Physics*, operating jointly with the neighboring Max Planck Institute for Chemical Physics of Solids (MPI-CPfS). Moreover, *Dr. K. Hornberger* arrived at the mpi**pks** to head the research group *Molecular Quantum Optics*. In the following year, *Prof. R. Ketzmerick* (TU Dresden) was appointed by the Max Planck Society as a *Max Planck Fellow* and started the activities of the Max Planck Fellow group *Quantum Chaos and Quantum Dynamics* at the mpi**pks**. In winter 2010, *Dr. E. Altmann* arrived to set up the Otto Hahn Group *Dynamical Systems and Social Dynamics*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* was renewed for a second six-year period.

2011-2012 • Further new groups were established: *Dr. F. Pollmann* set up the activities of the Junior Research Group *Topology and Correlations in Condensed Matter*, and *Dr. E. Gull* launched the Junior Research Group *Computational Quantum Many-Body Physics*. The group *Physics of the Cytoskeleton* headed by *Dr. G. Salbreux*, the group *Computational Biology and Evolutionary Genomics* headed by *Dr. M. Hiller*, and the group *Collective Dynamics of Cells* headed by *Dr. V. Zaburdaev* were installed to complement the activities of the *Biological Physics* division. Within the division *Finite Systems*, *Dr. A. Eisfeld* was appointed head of the group *Quantum Aggregates*, and *Dr. N. Rohringer* head of the group *X-Ray Quantum Optics*, which operated at the Center of Free-Electron Laser Science, Hamburg. To accommodate the increasing number of visiting scientists, a fourth guest house was built and inaugurated in November 2012. The joint research program of the mpi**pks** and the MPI-CBG was intensified and institutionalized in the form of the newly founded *Center for Systems Biology Dresden* (CSBD).

2013-06.2015 • During this period, the research at the mpi**pks** has once more acquired new foci due to the installation of new groups. *Dr. J. Bardarson* complements the Condensed Matter division as head of the group *Quantum Matter - Transport and Dynamics*, *Dr. A. Landsman* and her group *Ultrashort laser-matter interaction* add to the Finite Systems division, and *Dr. J. Brugués* and his group *Self-organization of biological structures* to the Biological Physics division and the CSBD. In 2015, the Max Planck Fellowship of *Prof. R. Ketzmerick* (TU Dresden) and his Max Planck Fellow Group *Quantum Chaos and Quantum Dynamics* were extended to a second five-year period by the Max Planck Society.

07.2015-2018 • Several new research groups began their scientific work at mpi**pks**. The Condensed Matter division is strengthened by the arrival of *Dr. M. Heyl*, heading the group *Dynamics in Correlated Quantum Matter*, and *Dr. D. Luitz*, heading the group *Computational Quantum Many-body Physics*. The Biological Physics division welcomes the groups of *Dr. S. Rulands* working on *Statistical Physics of Living Systems* and *Dr. C. Weber* who heads the group *Mesoscopic Physics of Life*. Moreover, the research profile of mpi**pks** is complemented by the establishment of three Max Planck Research groups, headed by *Dr. A. E. B. Nielsen*, who focuses on *Quantum Many-body Systems*, *Dr. F. Piazza*, studying *Strongly*

Correlated Light-Matter Systems and *Dr. I. A. N. Sodemann Villadiego* investigating *Fractionalization and Topology in Quantum Matter*. The International Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* successfully passed the 12-years evaluation in September 2015 and was renewed for another six-year period, with a new focus on *Many Particle Systems in Structured Environments*. The new building of the *Center for Systems Biology Dresden* was inaugurated in 2017. *Mrs. I. Auguszt*, who headed the administration of mpi**pks** since its foundation, retired in 2017, with *Mrs. K. Huppertz* taking over the responsibility as head of administration.

2019-09.2021 • A large part of this period was overshadowed by the global Covid 19 outbreak, which impeded the scientific life at the institute in both of its essential pillars - internal activities as well as the visitors program. In this period, a transition from exclusively in-person to virtual and hybrid meeting formats was commenced. Even in these difficult times, several groups have successfully concluded their work at the institute with the group leaders transitioning to faculty positions, while the in-house research activities were reinforced by new arrivals. Following the departure of Prof. Dr. Takashi Oka, the new joint research group *Correlations and Topology* between the mpi**pks** and the MPI-CPfS was founded and is headed by *Dr. A. Cook*. The Finite Systems division welcomes *Dr. M. Eiles* who heads the group *Correlations and Transport in Rydberg Matter*, while the arrival of *Dr. M. Popović* strengthens the Biological Physics division with the foundation of the group *Order and Disorder in Driven Systems*. The new Max Planck research group *Self-organization of Multicellular Systems* at the Center for Systems Biology Dresden is headed by *Dr. P. A. Haas* and further intensifies the collaborations between the mpi**pks** and the MPI-CBG.

10.2021-2024 • With the end of the pandemic, the workshop program at the institute returned to mostly in-person events, while the newly extended modern infrastructure of the seminar rooms enabled a novel workshop format with nodes on two different continents. A pilot event was held in summer 2024 jointly with the Center for Theoretical Physics of Complex Systems in Daejeon, Korea. The period is also marked by the establishment of seven new research groups within three years. *Dr. R. Alert* arrived in October 2021, heading the group *The Physics of Living Matter*. Three more groups followed in 2022, with *Dr. C. Kurzthaler* and her group *Transport and Flows in Complex Environments*, the group of *Dr. P. Claeys* working on *Dynamics of Quantum Information*, and *Dr. M. Bukov* establishing the group *Nonequilibrium Quantum Dynamics*. In 2023, the Emmy Noether Group of *Dr. A. Wietek* commenced their research on *Superconductivity and Magnetic Correlations*, and the mpi**pks** also welcomed *Prof. Dr. J. Budich* from the Technical University of Dresden as a new Max Planck Fellow, heading the group *Dissipative Quantum Matter*. The most recent arrival in 2024 was the foundation of the group *Functional Quantum Matter* of *Dr. L. Šmejkal*, which strengthens the collaborations between the mpi**pks** and the MPI-CPfS. Further new impulses are set by the appointment of *Prof. Dr. H. Harrington* as a new director at the MPI-CBG and her department *Algebraic Systems Biology*. Her arrival crucially reinforces the scientific activities at the Center for Systems Biology Dresden and the synergies between the mpi**pks** and the MPI-CBG. The International Max Planck Research School at the institute, which was founded in 2005 and since then funded in six-year-periods, has been installed permanently in 2023, with focus on *Quantum Dynamics and Control*. In 2023, mpi**pks** celebrated its 30th anniversary, which also marks 30 years of the Max Planck Society in Saxony. This milestone was publicly celebrated in Dresden and Leipzig and included a scientific workshop at the institute with contributions from many alumni. On April 11 2024, the founding director of mpi**pks** *Prof. Dr. P. Fulde* passed away shortly after his 88th birthday. In honor of his memory, a workshop on *Electronic Correlations and Beyond* was held at the institute in October 2024.

Present status of former group leaders

Research groups established 1995-2010

Group	Active	Leader	Current affiliation
Pattern Formation in Reaction-Diffusion-Systems	1995 - 2004	M. Bär	Head of Department PTB Berlin
Quantum Chaos and Mesoscopic Systems	1996 - 2001	K. Richter	Professor University of Regensburg
Quantum Chemistry (first period)	1996 - 2000	M. Dolg	Professor University of Cologne
Quantum Chemistry (second period)	2000 - 2005	U. Birkenheuer	Staff Scientist HZ Dresden-Rossendorf
Nonlinear Dynamics in Quantum Systems	1999 - 2007	A. Buchleitner	Professor University of Freiburg
Complex Media and Mesoscopic Phenomena	2000 - 2005	H. Schomerus	Professor Lancaster University
Physics of Biological and Soft Matter	2002 - 2006	R. Everaers	Professor ENS de Lyon
Biological Physics of Olfaction: From Genes to Networks	2002 - 2008	M. Zapotocky	Senior Scientist Czech Academy of Sciences
Nonlinear Processes in Strong Fields	2002 - 2008	A. Becker	Distinguished Professor & Fellow JILA Boulder, USA
Electronic Structure of Finite Systems	2003 - 2005	S. Kümmel	Professor University of Bayreuth
Physics of Cell Division	2004 - 2006	K. Kruse	Professor University of Geneva
Many Body Effects in Mesoscopic Systems	2006 - 2012	M. Hentschel	Professor TU Chemnitz
Motor Systems	2006 - 2013	S. Grill	Director MPI-CBG
Dynamics of Biological Networks	2007 - 2011	T. Gross	Professor University of Oldenburg
Stochastic Processes in Biophysics	2007 - 2011	B. Lindner	Professor HU Berlin
Computational Nonlinear and Relativistic Optics	2007 - 2014	S. Skupin	CNRS Researcher Université de Bordeaux
New States of Quantum Matter	2008 - 2011	A. Läuchli	Professor EPFL Lausanne
Complex Dynamics in Cold Gases	2008 - 2017	T. Pohl	Professor TU Vienna
Molecular Quantum Optics	2009 - 2011	K. Hornberger	Professor University of Duisburg-Essen
Collective Phenomena in Solid State and Materials Physics	2009 - 2014	S. Kirchner	Professor NYCU, Taiwan
Physics of the Cytoskeleton	2010 - 2015	G. Salbreux	Professor University of Geneva
Dynamical Systems and Social Dynamics	2010 - 2016	E. Altmann	Associate Professor University of Sydney

Research groups established since 2011

Group	Active	Leader	Current affiliation
X-Ray Quantum Optics	2011 - 2015	N. Rohringer	Professor University of Hamburg
Topology and Correlations in Condensed Matter	2011 - 2016	F. Pollmann	Professor TU Munich
Computational Biology and Evolutionary Genomics	2011 - 2021	M. Hiller	Professor University of Frankfurt
Computational Quantum Many-Body Physics	2012	E. Gull	Associate Professor University of Michigan
Collective Dynamics of Cells	2012 - 2018	V. Zaburdaev	Professor FAU Erlangen-Nuremberg
Quantum Matter - Transport and Dynamics	2013 - 2017	J. H. Bardarson	Assistant Professor KTH Stockholm
Self-Organization of Biological Structures	2013 - 2023	J. Brugués	Professor TU Dresden
Ultrafast Laser-Matter-Interactions	2014 - 2019	A. Landsman	Professor Ohio State University
Nonequilibrium Quantum Matter	2015 - 2020	T. Oka	Professor University of Tokyo
Quantum Many-Body Systems	2016 - 2021	A. E. B. Nielsen	Associate Professor Aarhus University
Dynamics in Correlated Quantum Matter	2016 - 2021	M. Heyl	Professor University of Augsburg
Fractionalization and Topology in Quantum Matter	2017 - 2022	I. Sodemann	Professor University of Leipzig
Statistical Physics of Living Systems	2017 - 2022	S. Rulands	Professor LMU Munich
Strongly Correlated Light-Matter Systems	2017 - 2024	F. Piazza	Professor University of Augsburg
Mesoscopic Physics of Life	2018 - 2021	C. A. Weber	Professor University of Augsburg
Computational Quantum Many-Body Physics	2018 - 2021	D. Luitz	Professor University of Bonn

1.2 Research Areas and Structure of the Institute

The institute investigates collective phenomena in classical and quantum physics. Its three divisions focus their research activities on the following main areas:

- With the help of quantum and semiclassical methods, the division *Finite Systems* headed by *Prof. J. M. Rost* focuses on the nonlinear dynamics of atoms, molecules and clusters.
- The division *Biological Physics* headed by *Prof. F. Jülicher* studies biological systems with tools of statistical physics and nonlinear dynamics.
- The division *Condensed Matter* headed by *Prof. R. Moessner* studies the classical and quantum statistical mechanics and dynamics of condensed matter.

The divisions are supplemented by research groups, which thematically expand, fortify and bridge the research activities:

- The research group *Nonlinear Time Series Analysis* headed by *Prof. H. Kantz* is the only permanent research group and analyzes temporal and spatial fluctuations in different kinds of deterministic and stochastic systems, with particular emphasis on climate dynamics.

- The research group *Quantum Aggregates* headed by *Dr. A. Eisfeld* investigates the emergence of collective effects in assemblies of atoms or molecules, with a particular focus on the coupling between electronic and nuclear degrees of freedom.
- The research group *Correlations and Topology* headed by *Dr. A. Cook* focuses on the search for novel phases of matter and exploration of mechanisms for experimental realization of exotic phases, and aims to accelerate the process of transitioning from the prediction of novel phases of matter in the literature to experimental realization.
- The research group *Correlations and Transport in Rydberg Matter* headed by *Dr. M. Eiles* aims to answer fundamental questions about atomic structure, low-energy collisions and scattering, and the behavior of ultracold gases via the study of Rydberg systems, while also raising new questions related to localization, transport, highly correlated systems, quantum chaos, semiclassical dynamics, and quantum simulation.
- The research group *Order and Disorder in Driven Systems* headed by *Dr. M. Popović* studies mechanical and rheological properties of out-of-equilibrium systems, with an emphasis on development of biological tissues and the role of structural disorder.
- The research group *Nonequilibrium Quantum Dynamics* headed by *Dr. M. Bukov* studies problems at the intersection of many-body dynamics, quantum simulation, quantum control, and applications of machine learning in physics, both on fundamental level and with relevance to immediate applications.
- The research group *Dynamics of Quantum Information* headed by *Dr. P. Claeys* is interested in the dynamics of quantum many-body systems, with special attention paid to the role of quantum information and entanglement.
- The Max Planck research group *Self-Organization in Multicellular Systems* headed by *Dr. P. A. Haas* develops the continuum mechanics of biological tissues in order to understand how biological robustness in development is compatible with mechanical constraints and biological variability.
- The Max Planck research group *Transport and Flows in Complex Environments* headed by *Dr. C. Kurzthaler* studies physical phenomena emerging from the interactions of cells, subcellular components, and inanimate materials with complex environments, through the lens of statistical physics and fluid mechanics.
- The Max Planck research group *Functional Quantum Matter* headed by *Dr. L. Šmejkal* covers a range of topics in quantum solid-state physics, focusing on unconventional magnets, such as altermagnets, topological materials, and quantum phases that arise from strong correlations and quantum coherence.
- The Max Planck research group *The Physics of Living Matter* headed by *Dr. R. Alert* aims to develop the physics of active matter to understand collective behaviors in cells and tissues.
- The Emmy Noether research group *Superconductivity and Magnetic Correlations* is headed by *Dr. A. Wietek* and aims at understanding how the macroscopic behavior of materials, like various forms of magnetism or superconductivity, emerges and investigates under which circumstances entirely new states of matter, like quantum spin liquids, can occur.
- The Max Planck Fellow group *Dissipative Quantum Matter* headed by *Prof. J. C. Budich* explores quantum many-body systems in which dissipation plays a crucial role, for example inducing novel phases of topological matter or enabling the controlled preparation of complex quantum states in the context of quantum simulators.

1.3 Workshop and Visitors Program

Its large program for visiting scientists makes the **mpipks** an almost unique institute within the Max Planck Society, comparable perhaps only to the MPI for Mathematics in Bonn. The visitors program administers individual stays for guest scientists at the institute (p. 125), but also international workshops and seminars (p. 136). For these, it offers both logistical and technical support, as well as access to facilities (seminar rooms, offices, guest houses).

Financial support for visits is open to scientists at all levels of their career, from students all the way to sabbatical support for professors. The duration of the stays varies between a few weeks to a maximum of two years. Financial support for visits, as well as funding for workshops, are awarded by two separate selection committees that include external experts as members.

Special programs include *Advanced Study Groups* (up to two per year) to foster the exchange between outstanding scientists and young researchers in residence (p. 47). Each group consists of several long-staying senior scientists and focuses on a current and important topic in the field of Complex Systems. The activities are reinforced by short-term visitors who join the group for seminars, lectures, discussions, and other meetings.

Since 2000, the mpi**pks** annually awards the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist (p. 126), who spends up to one academic year at the institute.
Moreover, the mpi**pks** annually offers one *Distinguished PKS Postdoctoral Fellowship* to an excellent young postdoc (p. 133).

Given the internationality and the rich interactions of the workshop and visitors program, the Covid-19 pandemic represented a severe setback for its activities, as it impeded two fundamental aspects of scientific life: The ability to travel and the ability to interact. Thus, the number of visiting scientists (including workshop participants) was lower than usual during the years 2021 and 2022, before returining to its normal values ranging between 1200 and 1700 in 2023 and 2024. During the pandemic years, the insitute built up the infrastructure required to organize vitual and hybrid workshops, which can now be used to offer remote options for the participants of a workshop, at the discretion of its scientific organizers. Furthermore, the concept for binodal workshops, in which two audiences in separate continents are virtually merged into a single event, was developed on the back of this infrastructure and implemented with the first event of this kind: The binodal intercontinental workshop and seminar "Flat bands and high-order Van Hove singularities", which took place between May 27 and June 7, 2024 and successfuly joined 73 participants at mpi**pks** with 74 participants at the Center for Theoretical Physics of Complex Systems of the Institute for Basic Science in Daejon, South Korea. Such a format will be further developed in the future and is particularly suitable for short events with a considerable fraction of overseas participants, as it eliminates the necessity for long-distance flights for just a few days of attendance and thus positively contributes to reducing the environmental footprint and enhancing the sustainability of our workshop program.

1.4 Teaching and Training

In addition to our core activities, we engage in teaching and training.

Training • The mpi**pks** runs the IMPRS *Quantum Dynamics and Control*, which was made permanent in 2023 and offers a structured PhD training framework (p. 13). It also participates in the IMPRS for *Cell, Developmental and Systems Biology* run by the MPI-CBG, which provides a similarly broad spectrum of lectures and courses. In addition, it is part of various third party funded structured graduate programs (p. 177).

Our PhD students and postdocs are admitted to lecture courses of the TU Dresden as well as events of the Workshop and Seminar Program (p. 143). In addition, the institute organizes soft skill training events such as German courses or a presentation series on professional skills and career coaching (p. 181). These are open to all junior scientists.

Teaching • Experienced postdocs and group leaders conduct lecture series at the TU Dresden and at other universities (p. 180). The benefit is mutual: The lectures offered often cover latest developments, thus complementing the standard curriculum; at the same time, our young researchers gain valuable teaching experience.

Research Organization • The large Workshop and Seminar Program at the mpi**pks** also offers young scientists the opportunity to gain experience in the organization of meetings. Thus, they can influence a broader research agenda and grow in visibility. Between September 2021 and December 2024, non-tenured junior scientists were involved in the coordination of almost half of all the events taking place under the umbrella of the visitors program (p. 143).

1.5 Diversity

The structure of the institute offers ideal conditions for the promotion of diversity. Via the unique flexibility of the visitors program, we are able to support stays of different lengths (from a few days to several years), and with different purposes (from workshop participation to collaborations, PhD training or sabbatical stays), logistically and/or financially as needed. In this way, we can tailor our support to individual needs, profiles, and backgrounds. On average the institute hosts scientists from about 40 countries at any given time.

The mpi**pks** is committed to promote the advancement of women in science. It participates in the annual *Girl's Day*, invites female students from high schools to lectures and discussions about a career in science, and encourages female scientists to apply for positions. Furthermore, 4 female scientists in residence volunteer to be listed as contact persons on the institute homepage as contacts for first-hand information about life and work at mpi**pks**, in particular as a woman scientist. The percentage of female researchers is currently 14% among postdocs and 16% among doctoral students.

To accommodate the requirements of researchers with small children the institute provides a *parent & child office* in one of the guest houses. It can be used by members of the mpi**pks** or short-term guests who might need to bring their children during working hours. Furthermore, a number of slots are reserved at two daycares nearby for children (from toddlers to pre-school age) of institute members.

1.6 Public Relations and Outreach

The institute endeavours to bring science, and our contribution to it, closer to the general public.

Each year, we reach about 2800 people with public evening lectures offered in connection with scientific workshops, the institute's activities at the *Long Night of the Sciences* (p. 184), and the lecture series *Science in the Theater* (p. 184).

A particular focus of the outreach efforts is to acquaint children and teenagers with the sciences and encourage them to approach scientific topics with confidence (p. 185): Our contributions to the program *Junior Doctor* aim to arouse the curiosity of young children in a playful way. The school contact program addresses high school students, whom we hope to inspire through direct contact with young researchers.

1.7 Research Networking

Local • The mpi**pks** finds itself in the midst of a rich research environment formed by the TU Dresden and the surrounding research institutes. The vivid scientific dialogue with the TU Dresden is mirrored in the Max Planck Fellow Group *Dissipative Quantum Matter* headed by *Prof. J. C. Budich* , as well as in the mpi**pks** participation in two clusters of excellence: *Physics of Life* and *Complexity and Topology in Quantum Materials*, respectively. Other joint initiatives include the collaborative research center *Correlated Magnetism: From Frustration To Topology*, the International Max Planck Research Schools for *Cell, Developmental and Systems Biology* and for *Quantum Dynamics and Control* (p. 13). The mpi**pks** has particularly close contacts to the Institute of Theoretical Physics of the TU Dresden and is involved in a number of joint projects (p. 177). Further collaborations with the TU Dresden include the Biotechnology Center (BIOTEC), the Center for Regenerative Therapies (CRTD), the Center for Molecular and Cellular Bioengineering (CMCB) and the Center for Molecular Bioengineering (BCUBE). The division *Biological Physics* is in close collaboration with the Max Planck Institute of Molecular Cell Biology and Genetics. The cooperation between both institutes has institutionalized in 2012 by the foundation of the intersectional Center for Systems Biology Dresden (p. 11). The division *Condensed Matter* cooperates with the Leibniz Institute for Solid State and Materials Research Dresden and with the neighbouring Max Planck Institute for the Chemical Physics of Solids, specifically through joint research groups (p. 13).

National and International • The numerous different national and international collaborations and contacts are listed in the research group reports (Chapters 1.8 – 1.11, and 3.4).

1.7.1 Center for Systems Biology Dresden

The Center for Systems Biology Dresden (CSBD, https://www.csbdresden.de) is jointly operated by the mpi**pks** and the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), in collaboration with the Technical University Dresden (TUD). The center was established in 2012 as an intersectional operation of the Max Planck Society. Its creation resulted from the strong track record of the joint research program of MPI-CBG and mpi**pks** on the Physics of Biological Systems, that had been initiated a decade earlier.

Eugene Myers was recruited in 2012 as a director at MPI-CBG. With his focus on bioinformatics, genomics and image informatics combined with the development of novel microscopy techniques, he brought a strong computer science program to the CSBD. Ivo Sbalzarini develops computational biology approaches to image based systems biology. He also started in 2012 as a professor at TUD and a group leader at MPI-CBG. A new building, funded by the Free state of Saxony, was inaugurated in 2017. It hosts several research groups conducting theoretical and computational research in Physics, Mathematics and Computer Science with tight links to Biology. In order to integrate different disciplines, the CSBD operates the ELBE postdoc program, attracting postdocs who bridge between theory and experiment and are affiliated with typically two groups from different disciplines. The ELBE postdoc program is administered by mpi**pks**.

Eugene Myers retired in 2022. He is succeeded by Heather Harrington who joined in 2023 from the University of Oxford. Prof. Harrington heads a department on Mathematics for Biology at MPI-CBG with her research group being located in the CSBD. She develops novel approaches to data science, with a particular focus on topological data analysis and she brings mathematical concepts to the analysis of biological data. With the hire of Heather Harrington, the CSBD now is joining forces of Mathematics, Computer Science and theoretical Physics to advance challenges in biology, providing a very stimulating and interactive environment in the coming years.

Research at the CSBD studies integrated biological systems and processes using computational and theoretical approaches in close collaboration with experiments. The center serves as a hub and intellectual incubator that brings physicists, mathematicians, computer scientists, together with biologists at the nearby MPI-CBG, aiming at a quantitative understanding of dynamic processes and spatiotemporal organization in living systems. The MPI-CBG has the research theme "How do cells form tissues?". Understanding the principles of cellular and tissue organization requires the study of collective effects and emergent phenomena. Molecules organize collectively in cells and cells organize collectively in tissues. Research at the center investigates the principles underlying system behaviors and spatiotemporal processes. For example the question how tens of thousands of cells coordinate their behavior in space and time to form tissues of a given form and function. To answer such questions, we combine a unique blend of theoretical and computational approaches. With the addition of mathematics since the arrival of Heather Harrington, a new focus is data science such as topological data analysis, which is a multi-scale approach to identify and characterize topological features in complex data.

Scientists at the CSBD work in a melting pot of the different scientific environments and speak the language of different disciplines. PhD students and postdoctoral researchers typically have a background in one discipline. A key mission of the CSBD is to train PhD students and postdoctoral researchers to conduct research projects that reach out to other fields. To this end, the ELBE postdoc program has been established. The ELBE postdoc program attracts postdoctoral researchers that work across disciplines from physics and computer science to biology and between experiment and theory. This program is modelled on the visitors program of mpi**pks** and is administered by mpi**pks**. The ELBE postdoc program also stimulates collaborations between experimentalists and theorists. Therefore, ELBE postdocs are usually affiliated with two research groups, typically one experimental and one theoretical. Furthermore, the Center also organizes the ELBE PhD track that funds PhD students that carry out projects across disciplines.

Operations of the center are managed by a steering committee. It has representatives of both Max

Planck Institutes and it is responsible for deciding upon the scientific vision, profile of research activities, programs and technologies, as well as overseeing the allocation of shared resources (space, equipment, personnel, CSBD funds). Only CSBD members serve on the Steering Committee. Furthermore, a CSBD Coordinator is responsible for external and internal communications of the CSBD, particularly ensuring the communication flow between the participating institutions. In addition, the coordinator supports the Steering Committee by enacting many of the decisions made.

Members of the center are research groups affiliated with MPI-CBG and **mpipks**. Groups that use office space in the CSBD building are

- Ricard Alert, (**mpipks**): The physics of living matter
- Pierre Haas, (**mpipks** and MPI-CBG): Self-organization of multicellular systems
- Heather Harrinton, (MPI-CBG): Algebraic Systems Biology
- Frank Jülicher, (**mpipks**): Theory of biological systems
- Aida Maraj, (MPI-CBG): Algebra in Data Analysis
- Carl Modes, (MPI-CBG): Network complexity and systems biophysics
- Türkü Özlüm Celik, (MPI-CBG): Mathematical Structures and Applications
- Eugene Myers, (MPI-CBG): Exploring cells and systems via image analysis, customized microscopy, and genomics (until 2022)
- Ivo Sbalzarini, (MPI-CBG and TU Dresden): Scientific computing for image-based systems biology
- Agnes Toth-Petroczy, (MPI-CBG): Protein plasticity and evolution
- Christoph Zechner, (MPI-CBG): Stochastic models of molecular networks (until 2024)

Furthermore, there is an additional depth in physics, computer science and biology brought by the following research groups that are involved in the governance and research of the CSBD as members: Jan Brugués (TUD), Stephan Grill (MPI-CBG), Tony Hyman (MPI-CBG), Christina Kurzthaler (**mpipks**) Marko Popović (**mpipks**), Steffen Rulands (**mpipks**, until 2022), Pavel Tomancak (MPI-CBG), and Marino Zerial (MPI-CBG, until 2024). The program is further strengthened by its close involvement with all the researchers of the MPI-CBG, **mpipks**, and the following additional CSBD affiliates: Björn Andres (TU Dresden), Stefan Diez (TU Dresden), Benjamin Friedrich (TU Dresden), Anna Pötsch (TU Dresden) and Axel Voigt (TU Dresden). Moreover, the CSBD has established a good relationship with the faculties of Physics, of Mathematics and of Computer Science at the TU Dresden and with the biotechnology center, as well as with the Cluster of Excellence Physics of Life.



The Center for Systems Biology Dresden (CSBD) is jointly operated my **mpipks** and MPI-CBG in cooperation with the Technical University Dresden (TUD). Several computational and theory groups of the CSBD are accommodated in a building that was inaugurated in 2017. The building is located next to the MPI-CBG and provides a stimulating environment for physicists, mathematicians and computer scientists that facilitates interactions between theory and research in cell and developmental biology. Pictures by Jussi Tiainen.

1.7.2 Joint research group with MPI-CPfS

One of the main research themes of **mpipks** is the study of condensed matter physics, specifically at the intersection with materials physics. This was central to Peter Fulde's Strongly Correlated Electron Systems Division, and it has continued seamlessly into the present through the activities of the Condensed Matter Division.

In this context, the institute benefits from the experimental research activities of the neighbouring Max Planck Institute for the Chemical Physics of Solids (MPI-CPfS). MPI-CPfS pursues an interdisciplinary approach to materials physics, linking a broad spectrum of approaches from chemistry and physics, with directors Yuri Grin (Chemical Metals Science), Hao Tjeng (Physics of Correlated Matter), Claudia Felser (Topological Quantum Chemistry) and Andrew Mackenzie (Physics of Quantum Materials).

The two institutes collaborate in various ways, both on an ad-hoc basis as well as in a more structured fashion. The backbone of the latter is provided by a joint theory research group. Its purpose is to facilitate communication and collaborations between the two institutes. This enables members of both institutes to join forces in studying strongly correlated electron physics, superconductivity and magnetism. The head of the current group "Correlations and Topology" is Ashley Cook, who succeeded Takashi Oka after his move to a professorship at the Institute for Solid State Physics at the University of Tokyo. This has been further reinforced by the arrival of Libor Šmejkal in 2024, whose group "Functional Quantum Matter" is also affiliated with both institutes.

Both institutes are also involved in large-scale collaborative initiatives, such as in the Collaborative Research Centre "Correlated Magnetism: from Frustration to Topology" and the Cluster of Excellence "Complexity and Topology in Quantum Matter". In parallel, the ad-hoc collaborations exist on subjects such as electronic transport in ultraclean electronic systems. This includes electronic hydrodynamics, a topic extending existing efforts at the institute which reaches deep into the biophysical research carried out here.

1.7.3 International Max Planck Research School

International Max Planck Research Schools (IMPRS) are structured doctoral programs intended to attract talented students from around the world. Currently, there are 68 IMPRS within the Max Planck Society across a wide range of topics where English is the working language. The IMPRS infrastructure involves collaborations with national as well as international universities and research institutions. This provides a vibrant and versatile scientific environment that offers to the students the possibility for interdisciplinary research projects.

The IMPRS headquartered at **mpipks** was established in 2005 and ran successfully for three six-year periods:

- **2005-2010 & 2011-2016**: Focusing on Dynamical Processes in Atoms, Molecules and Solids. In these two funding periods the IMPRS was restructured addressing the ever changing tendencies of the research landscape - including the establishment of an IMPRS at the neighbouring MPI for Chemical Physics of Solids.
- **2017-2022**: Focusing on Many-Particle Systems in Structured Environments. In this funding period the IMPRS provided a new research trajectory reflecting the growing importance of open many-body systems on a fundamental level as well as on the experimental realizations of quantum devices

Since 2023 the IMPRS acquires permanent status after a successful evaluation at the end of 2022. The current iteration of the IMPRS has a focus on Quantum Dynamics and Control, facilitating two main and overlapping research thrusts: (i) the dynamics of few to many-body systems interacting with an environment and (ii) their control towards effective use for quantum information and other purposes.

Research areas include (i) emergent collective phenomena in Rydberg atomic ensembles, solid state materials embedded in optical cavities, organic molecules in solution, nuclear matter at high temperature and density or in exotic quantum many-body phases under (periodic) driving. Relevant topics of quantum control include (ii) state-to-state manipulation of quantum systems and the mitigation of environmental effects with the goal of new research possibilities in experimentally challenging regimes, such as the development of quantum simulators and ultimately quantum computers. Each of these areas presents

new questions and exciting opportunities for young researchers. Members of the IMPRS find themselves part of an active research community, both within the graduate school and, partly through events that the school organizes, they are exposed to the frontiers of all these topics, of course alongside carrying out original research for their PhD thesis.

The location of mpi**pks** in the immediate vicinity of Poland and the Czech Republic made it possible for the IMPRS to be established on the strength of international research collaborations in three different countries. In particular, the IMPRS for Quantum Dynamics and Control is comprised of research groups at the follow institutions:

1. Max Planck Institute for the Physics of Complex Systems - mpi**pks**
2. Technische Universität Dresden - TUD
3. Leibniz Institute for Solid State and Materials Research - IFW (Dresden, Germany)
4. Institute of Low Temperature and Structure Research - ILTSR (Polish Academy of Sciences, Wrocław, Poland)
5. University of Wrocław
6. Wrocław University of Science and Technology
7. Institute of Organic Chemistry and Biochemistry - IOCB (Prague, Czech Republic)
8. University of Chemistry and Technology - UCT (Prague, Czech Republic)
9. Charles University (Prague, Czech Republic)

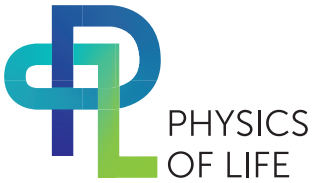
The school has 28 partners who make up the IMPRS board including one coordinator and 27 who act as PhD advisors for students of the graduate school. All matters concerning the large-scale operation of the graduate school are decided in the board meetings including the admission of new students, the allocation of IMPRS funds, the program of IMPRS events including the summer school and retreat.

- Prof. A. Bäcker (TUD)
- Prof. D. Blaschke (University of Wrocław)
- Prof. J. Budich* (TUD)
- Prof. B. Büchner (IFW)
- Dr. M. Bukov (mpi**pks**)
- Dr. P. Claeys (mpi**pks**)
- Dr. A. Cook (mpi**pks**)
- Prof. G. Cuniberti (TUD)
- Dr. M. Eiles (mpi**pks**)
- Dr. A. Eisfeld (mpi**pks**)
- Dr. P. Giannakeas* (coordinator, mpi**pks**)
- Prof. F. Großmann (TUD)
- Dr. M. Haque (TUD)
- Prof. T. Heine (TUD)
- Prof. P. Jungwirth (IOCB)
- Prof. R. Ketzmerick* (TUD)
- Prof. O. Marsalek (Charles University)
- Prof. R. Moessner* (mpi**pks**)
- Dr. F. Piazza (mpi**pks**→ University of Augsburg)
- Prof. J.-M. Rost* (chairman, mpi**pks**)
- Prof. U. Saalmann (mpi**pks**)
- Prof. A. Sedrakian (University of Wrocław)
- Prof. P. Slavicek* (UCT)
- Dr. I. Sodemann (mpi**pks**→ Leipzig University)
- Prof. W. Strunz (TUD)
- Prof. P. Surowka (Wrocław University of Science and Technologies)
- Dr. A. Wietek* (mpi**pks**)
- Prof. T. Zaleski* (ILTSR)

There is a board composed of some subset of the partners (asterisked) that meets approximately once per year.

There is an executive board composed of the chairman, coordinator and Prof. J. Budich that meets biannually to carry out an initial evaluation of new PhD applications.

1.7.4 Cluster of Excellence: Physics of Life



The Cluster of Excellence Physics of Life (PoL, https://physics-of-life.tu-dresden.de) was established in 2019 at the Technical University Dresden (TUD) in close cooperation with partner institutions in Dresden. It was selected in the German Excellence Strategy for the funding period 2019-2025. The concept of the cluster was developed jointly by scientists at the Max-Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) and at **mpipks**, with Stephan Grill as founding speaker. The cluster brings together principal investigators from TU Dresden and from several research institutions in Dresden with the aim to build a strong research environment on the Physics of Life at TUD, to broaden the scientific environment in Dresden at the interface between Physics and Biology. The scientific concept is to approach biological systems as physical systems and to elucidate laws of physics that underlie the dynamic spatiotemporal organization of life into molecules, cells and tissues. A key aim is to bring fundamental physics to biology for the purpose of solving biological questions. The cluster brings new professorships, new experimental methods and technologies as well as new approaches in scientific computating and systems microscopy to TUD. The research of the cluster integrates theory and experiment and different disciplines, driven by a sparkling collaborative atmosphere in Dresden between University and non-University research institutions.

Four full professorships (W3) and six junior group leaders have recently been recruited at PoL. These new groups create a strong pillar of research on the physics of life at the Technical University Dresden with broad visibility. The full professor hires are:

- Otger Campàs (formerly at UC Santa Barbara, USA). He works on the experimental physics of embryonic self-organization. Since 2023 he is the speaker of the Cluster of Excellence.
- Helmut Schiessel (formerly at Leiden University, Netherlands). He holds a professorship on the theoretical physics of living matter.
- Miki Ebisuya (formerly EMBL Barcelona, Spain). She studies how the timing of biological processes varies between species
- Jan Brugués (formerly **mpipks** and MPI-CBG). He investigates the self-organization of mesoscopic cellular structures.

New appointments of tenure track group leaders are Benjamin Friedrich, with a research focus on Biological algorithms; Elisabeth Fischer-Friedrich studying the biophysics of cell and tissues; Rita Matheus (formerly at University of Geneva, Switzerland) focussing on biophysical principles of growth and regeneration; Ellen Adams (formerly at Ruhr-Universität Bochum, Germany) with a research profile on the physical chemistry of soft biological matter; Xingbo Wang (formerly Harvard University, USA) investigating cellular and organismal energetics; and Elias Barriga (formerly Gulbenkian Institute, Lisbon, Portugal), investigating the biophysics of morpohogenesis and the role of electric fields in these processes.

In the future, the recently recruited groups will be accommodated in a new building that is currently in the planning phase. Based on a successful first funding period, a proposal for the next funding period 2026-2032 has been submitted in 2024 and is evaluated in 2025. The Cluster of Excellence Physics of Life provides a thriving research environment for scientists and postdocs from various disciplines, as well as a training ground for undergraduate and graduate students as well as for PhD students. A new master degree course Physics of Life has been established. The Cluster of Excellence Physics of Life is closely integrated with the joint research program of **mpipks** and MPI-CBG at the interface between Physics and Biology. It strengthens the local research environment in particular by bringing new experimental biophysics approaches to Dresden. These are in particular techniques for the measurment of mechanical stresses and osmotic pressures inside living tissues, techniques to measure metabolic flux with spatial resolution and the study of electric fields in tissues and their role in tissue regeneration and during development.

1.7.5 Cluster of Excellence: Complexity and Topology in Quantum Matter

The cluster of excellence Complexity and Topology in Quantum Matter (ct.qmat, https://www.ctqmat.de) is a collaborative research structure based in Dresden and Würzburg. It pursues an integrated research strategy, in which researchers from the fields of physics, chemistry and materials science cooperate to understand, control and apply topological states of quantum matter.

The study of topological phenomena has been one of the central themes of modern condensed matter physics, ever since the groundbreaking discovery of the quantum Hall effect by von Klitzing forty years ago. Indeed, two locations from which recent important contributions to this field in Germany have originated are Würzburg (observation of quantum spin Hall effect) and Dresden (prediction of magnetic monopoles in spin ice). At present, both **mpipks** and the Max Planck Institute for the Chemical Physics of Solids have strong research programmes in the field. These range from detailed materials modelling to the transfer of field theoretic insights from high-energy physics.

The cluster of excellence is organised into four research areas: topological electrons, quantum magnetism, topological photonics, and tailoring topological functionality. Functioning as a platform for exchange (including teaching) and collaborations, it provides funding for student and postdoctoral researchers as well as experimental projects.

The cluster has strengthened the research efforts in Dresden and Würzburg in the long term, in particular with the appointment of new professorships in the field. As one of three clusters of excellence in Dresden, it underpins the 'official' excellence status of the Technical University of Dresden. The funding for the cluster runs until the end of the year 2025. A renewal is possible, with an evaluation of the cluster having taken place in December 2024. The decision about the renewal of existing and establishment of new clusters of excellence will collectively be announced in late May 2025.

1.8 Divisions and Groups

Division: Condensed Matter
(Head: Prof. Roderich Moessner)

Condensed matter physics deals with physical processes and phenomena on many scales and levels, from their microscopic basis all the way to applications in daily life. One of its central attractions lies in the possibility of pursuing a research programme covering, and linking, many of these. In this spirit, the condensed matter division studies the collective behaviour of inanimate matter.

One focus of our work is the extension of the reach of equilibrium statistical mechanics, in particular into the topological realm as well as for the description of classes of computational problems. The aim is to identify qualitatively new phenomena, to develop their theoretical description alongside a conceptual framework, and to link them with experiment and/or simulation and computation. Magnetic systems have been particularly productive here, in their dual role as simple model systems as well as their manifold realisations in materials physics. Indeed, the Nobel Prize for John Hopfield has illustrated yet again the vast interdisciplinary reach of magnetic models. A further interdisciplinary impetus has been provided by the huge research (and commercial) effort to realise functional quantum computing platforms. The promise of controlled accessibility of a wide variety of ingredients, such as quantum coherence, driving protocols, or various forms of quenched disorder, has led to the discovery of a plethora of interesting phenomena and insights.

The following provides a barebones list of selected research highlights.

Non-equilibrium and non-linear dynamics: We have studied, both in theory and collaboration with experiment, the role of temporal disorder in a driven system, coining the concept of a partial 'rondeau' spatiotemporal form of order. We have demonstrated the existence of inverted many-body scars, highly-entangled states embedded in a sea of low-entangled states. In a separate thread, we have uncovered a remarkably rich phenomenology of anomalous transport phenomena in classical spin chains, including a KPZ regime for a Heisenberg ferromagnet, and the coexistence of nonlinear effects such as fragmentation of domain walls with a strongly-nonlinear regime captured by *linear* spin wave theory. We have identified a *'ballistic'* transport regime in a driven *disordered* spin chain. We have also initiated the study of hardcore spin models, in analogy to the study of hard spheres or rods, and analysed their jamming behaviour.

Quantum computing: Unlike in the case of classical computers, the power of present-day quantum computing platforms is not dominantly linked by limits imposed by run-time: the quality of the computation degrades on short timescales. Consequently, a primary optimisation goal is the minimisation of the number of (gate) operations, even if this optimisation is a costly process. We have developed an 'interactive' Trotterisation scheme where the output of a quantum computation is fed back into its own optimisation. We have also proposed a new construction for an 'entanglemon' q-bit architecture incorporating passive error correction.

Lifting topological censorship: The robustness of topologically protected observables renders much information about their microscopic realisation inaccessible. The development of local probes is opening a new window on this information, and following an experiment on the spatial current distribution in a Chern insulator, we have developed a detailed theory of generic transport regimes and their continuous tunability.

Search for, and properties of, spin liquids: We support progress of a large experimental search effort for materials realisations of spin liquids by method developments improving the modelling of three-dimensional quantum magnets. We use these on a growing body of experimental data to pinpoint which experimental compounds are located at or near spin liquid regimes on model phase diagrams. We have also studied the unconventional coupling of electromagnetic fields to emergent gauge fields, identifying new Nernst-type effects as well as novel hybrid dyons, quasiparticles carrying combinations of emergent and (Maxwell) electromagnetic charges. We have shown the emergence of a dynamical fractal in experiments on a *clean* topological magnet, identifying a mechanism for subdiffusion in three-dimensions, in absence of disorder.

Classification schemes: We have continued to develop classification schemes for classical spin liquids, which has in turn led to the identification of new spin liquids, whose properties are as yet largely unexplored. We have built on the classification of magnetic topological quantum chemistry with a classification of spin-space groups as well as finite-range tight-binding models. This has included the identification of topological magnon bands, e.g. in neutron scattering experiments on elemental Gd.

Perspectives. The development of the condensed matter division of **mpipks** has continued to be dynamic. Marin Bukov (2021), Pieter Claeys (2022), Ashley Cook (2020), Libor Šmejkal (2024) and Alexander Wietek (2022) have arrived after the departure of the group leaders Markus Heyl, David Luitz, Anne Nielsen, Takashi Oka, and Inti Sodemann, all of who have taken up professorships elsewhere. The long-standing collaboration with MPI-CPfS continues, with both Ashley Cook and Libor Šmejkal heading groups associated with both institutes.

Many-body dynamics in and out of equilibrium across timescales, ranging from early-time relaxation to late-time phenomena such as coarsening and glassiness will continue to be a central topic of study. This is a rich and rapidly moving field, driven by advances of various experimental platforms in materials physics and artificial systems, including quantum computing platforms.

On the materials physics front, the rich phenomenology of interacting topological phases will be a central research theme. The intersection with dynamical phenomena is considerable, in particular in the context of disordered topological systems, as well as in novel topological systems exhibiting reduced mobility defects.

Embedding in local research landscape. The condensed matter division is actively involved in a number of cooperative grants. The oldest is the collaborative research center SFB 1143 at TU Dresden, entitled "Correlated magnetism: from frustration to topology", which has successfully been renewed for a third (and final) funding period. The largest is the cluster of excellence ct.qmat — "complexity and topology in quantum matter" described in more detail above. Finally, there is the DFG Forschergruppe (research unit of the German Science Foundation) "Quantum thermalization, localization, and constrained dynamics with interacting ultracold atoms". Constituted in 2023, it joins and promotes research activities across Germany (Augsburg, Dresden, Göttingen, Munich and Tübingen).

Selected cooperations with theory groups internationally

- China: Peking University (Hongzheng Zhao)
- France: CEA Grenoble (Mike Zhitomirsky); École Normale Supérieure Lyon (Peter Holdsworth); Sorbonne Université Paris (Benoît Douçot); Cergy-Pontoise (Dmitry Kovrizhin)
- Great Britain: University of Cambridge (Claudio Castelnovo)
- Hungary: Budapest University of Technology and Economics (Balázs Dóra)
- India: IACS Kolkata (Arnab Das); Indian Institute of Science (Vijay Shenoy); Tata Institute for Fundamental Research (Subhro Bhattacharjee, Sthitadhi Roy)
- Italy: ICTP Trieste (Antonello Scardicchio)
- Japan: Gakushuin University (Masafumi Udagawa)
- United States: Boston University (Chris Laumann); Cornell University (Eun-Ah Kim); Stanford University (Vedika Khemani).

Selected cooperations with experimental groups

- Argentina: UNLP-Conicet La Plata – Santiago Grigera (non-equilibrium behaviour in spin ice)
- Canada: McMaster University – Bruce Gaulin (quantum spin liquids); UBC – Doug Bonn (transport in ultra-pure metals)
- Germany: High-magnetic field laboratory Dresden-Rossendorf – Hannes Kühne (field-tunable Kosterlitz-Thouless transition); MPI-CPfS– Andy Mackenzie (electron transport); MPQ – Johannes Zeiher/Immanuel Bloch (non-equilibrium dynamics); Uni Würzburg – Hendrik Bentmann (orbital vortex lines)
- United States: Google Quantum AI – Pedram Roushan (noisy intermediate scale quantum computing); John Hopkins University – Collin Broholm (magnetic mateials); Oak Ridge National Laboratory – Steve Nagler (magnetic materials).

Research Group: Dynamics of Quantum Information
(since June 2022, Head: Dr. Pieter W. Claeys)

The research group *Dynamics of Quantum Information* was established in June 2022 and studies the dynamics of quantum many-body systems, with special attention paid to the role of quantum information and entanglement. The group's research is motivated by theoretical and experimental developments in the rapidly developing field of quantum computation and simulation. This research lies at the interface of condensed matter physics and quantum information, approaching the quantum many-body problem using a variety of theoretical and numerical approaches. The group currently consists of four PhD students (Gabriel O. Alves, Michael A. Rampp, Philippe Suchsland, Jiangtian Yao) and four postdocs (Wouter Buijsman, Felix Fritzsch, Suhail A. Rather, Hansveer Singh), and has also hosted two summer internships (Agnieszka Wierzchucka, Oxford University, and Sean Casey, University College Dublin). Here we outline our main research topics.

Unitary circuit dynamics. Quantum circuits originate from quantum computation and have recently become a fruitful playground for the theoretical and experimental study of many-body dynamics. In such circuits a quantum state is evolved through the repeated application of unitary gates, building up entanglement and mimicking Hamiltonian dynamics in a discrete time. On the theoretical side, minimal circuit models can be developed that allow for analytical insights in universal aspects of many-body dynamics by either fine-tuning or randomizing the constituting gates. On the experimental side, digital

quantum simulators natively realize such architectures and allow for precise control over a large number of quantum degrees of freedom, making them ideal experimental testbeds for circuit dynamics.

Our group has developed effective theories for the scrambling of quantum information in structured unitary circuits, elucidating the role of the entangling properties of the gates, and has developed various classes of circuits in which dynamical quantities could be fully characterized. While a full characterization of these quantities in many-body systems is in general exponentially costly, we developed theoretical tools that circumvent the quantum many-body problem by exploiting symmetries in space-time. In the resulting dual-unitary or multi-unitary circuits we recovered tractable dynamics of correlation functions, entanglement, and scrambling, applicable to wide classes of circuits with theoretical and experimental relevance. We unified different constructions of solvable circuits with (hierarchical) dual-unitary and triunitarity. We studied the dynamics of Hilbert space delocalization, the entanglement membrane, and the interplay of unitary dynamics with projective measurements in (temporal) entanglement. Quantum many-body systems remain highly complicated, and these analytical models presented important tools shedding light on various aspects of quantum many-body dynamics.

Novel probes of quantum ergodicity and universality. Current quantum simulation platforms allow for direct access to dynamical signatures going beyond standard correlation functions. The dynamics of these correlation functions and how these approach (thermal) equilibrium directly connects to statistical physics, and the question of how many-body dynamics recovers thermalization has been a fruitful field of study. These experimental advances now allow for the exploration of novel probes of quantum ergodicity, going beyond the standard paradigm of thermalization and the corresponding theoretical framework of the eigenstate thermalization hypothesis.

Our group has developed the theoretical framework of Krylov complexity for unitary dynamics and identified both universal signatures of maximal ergodicity and nonanalytical Trotter transitions in the Krylov dynamics. We presented exact results on the use of Hayden-Preskill information recovery protocols as dynamical probes of chaotic and integrable behavior and highlighted their sensitivity to characteristic dynamical features such as long-lived quasiparticles or dual-unitarity. Various extensions exist of the notion of thermalization, and our group constructed minimal models of 'deep' thermalization, encoding additional system-environment correlations, and 'full' eigenstate thermalization, describing higher-point correlation functions. These results provided theoretical insight in different notions of of ergodicity and helped uncover emergent universal dynamical behavior in a wide range of experimentally relevant models.

Many-body dynamics mediated by a central mode. The dynamics in lattice models is underlaid by locality, a crucial element in both our understanding and any physical theory of their dynamics. However, systems in which the interactions are mediated through a central mode lack a notion of locality and require a different understanding of their dynamics. These models are relevant for experimental platforms of quantum simulation including in cavity quantum electrodynamics, an important platform for quantum optics, as well as in platforms for quantum engineering such as nitrogen-vacancy centers in diamonds and solid-state quantum dots.

Our group has identified exactly solvable limits of the corresponding central spin models and the paradigmatic Tavis-Cummings model of quantum optics, uncovering hidden symmetries leading to integrability and presenting constructions for their exact eigenstates. In all such models the eigenstates were shown to exhibit anomalous localization properties, characterized by multifractality and semilocalization, which were directly related to experimentally accessible dynamical signatures of their models. We additionally studied the stability of these eigenstates and their localization properties, and developed control protocols that exploited the emergent Dicke symmetry in the closely related models with long-range interactions.

Collaborations

- Profs. Austen Lamacraft and Jamie Vicary (University of Cambridge, U.K.)
- Profs. Anushya Chandran, Chris Laumann, and Anatoli Polkovnikov (Boston University, U.S.A.)
- Prof. Siddharth Parameswaran (Oxford University, U.K.)
- Prof. Francesco Piazza (University of Augsburg, Germany)
- Prof. Giuseppe De Tomasi (University of Lisbon, Portugal)
- Prof. Sthitadhi Roy (International Centre for Theoretical Sciences, India)

Awards of people in the group

- Felix Fritzsch: Marie Curie Fellowship
- Michael A. Rampp: Participated in the 73rd Lindau Nobel Laureate Meeting

Research Group: Correlations and Topology
(Head: Dr. Ashley Cook)

The Correlations and Topology group focuses on the interplay between correlation effects in electronic systems and their relation to topologically-nontrivial phases of matter, or those phases of matter unaffected by sufficiently small perturbations. In particular, the group specializes in introducing novel topological phases of matter into the literature. While topological phases of matter were first studied in earnest in the early 1980's with discovery of the integer quantum Hall effect, the group has made significant advances by returning to the foundations of this area of research. This work of the group has culminated in generalisation of the framework of the quantum Hall effect to that of the quantum skyrmion Hall effect, by generalising interpretation and treatment of spin in quantum mechanics. Essentially, spin in quantum systems is encoded via matrix mechanics, with spin traditionally being interpreted as a label for quantum states. More recently, spin has instead encoded a finite number of spatial dimensions within non-commutative field theories, when spin is associated with matrix representations of size $N \times N$, where N is large, while spin is still assumed to encode only labels of quantum states for N small. However, within the framework of the quantum skyrmion Hall effect, spin is more accurately understood as encoding a finite number d of spatial dimensions both when N is large but also when N is small. Correspondingly, spin is more accurately described in terms of a severely-discretized, non-commutative, d+1 dimensional (+1 corresponds to the time dimension) gauge theory for $N \geq 2$. Furthermore, the group has re-examined past experiments and identified potential first experimental confirmation of the quantum skyrmion Hall effect.

Given the fundamental discovery of the quantum skyrmion Hall effect at the heart of the research group, there are now two major directions of research within it:

- First, the group continues to characterize the three sets of topological states leading to discovery of the quantum skyrmion Hall effect, using both analytical and numerical techniques to study this physics in lattice models. As each set contains a generalisation of the canonical Chern insulator phase, and the Chern insulator is traditionally the starting point in introduction and characterisation of a vast array of topological states even for effectively non-interacting systems in equilibrium, each set can be extended similarly, first by introduction and characterisation of related topological states for effectively non-interacting systems in equilibrium. These states can then be utilized to generalise to interacting counterpart topological states, analogous states of myriad quasiparticles, such as magnonic or phononic topological states, and also counterpart topological states of driven and open systems, such as Floquet and non-Hermitian variants. Myriad hybrid states are also possible, such as finite-size topological states which are also topological skyrmion phases of matter, in the sense that a layer (pseudo)spin degree of freedom important for a finite-size topological phase can be re-interpreted and treated as some other (pseudo)spin degree of freedom.
- The second major direction of work within the research group involves understanding the implications of this generalisation of spin angular momentum for quantum field theory, focusing in particular on long-standing challenges of quantum information, condensed matter, and high-energy physics. Spin angular momentum, even for small spin such as spin half, is more accurately described in terms of a severely-discretized gauge theory defined over a fuzzy coset space. This has profound implications for quantum computation and may address key paradoxical aspects of quantum mechanics such as the measurement problem, given this generalisation of spin amounts to uncovering of a century-old assumption on the treatment and interpretation of spin angular momentum. In condensed matter theory, the quantum skyrmion Hall effect implies the gauge theory at the heart of understanding unconventional superconductivity and quantum spin liquids, the 2+1 dimensional SU(2) gauge theory, must be generalised to include effectively higher-dimensional terms, which also play the role of dynamical gauge fields within the quantum skyrmion Hall effect. This will provide valuable insight into the mechanisms of unconventional superconductivity, which the community has pursued for the past four decades. Finally, some of the most promising attempts to unify the

four forces of nature are based on string theory, in which a key paradox is the need for more than four space-time dimensions. The quantum skyrmion Hall effect resolves this paradox by showing how the additional spatial dimensions of string theory might simply be understood as the spatial dimensions associated with myriad isospin degrees of freedom. The quantum skyrmion Hall effect also suggests that, rather than generalising particles as strings, a more physically meaningful possibility for generalising particles is as the truly quantum skyrmions of the quantum skyrmion Hall effect.

Research Group: Nonequilibrium Quantum Dynamics
(since September 2022, Head: Dr. Marin Bukov)

The Nonequilibrium Quantum Dynamics group was established in September 2022, and investigates the behavior of few- and many-particle systems out of equilibrium. The primary applications of our research are in quantum simulators and quantum computers, which operate away from equilibrium. Our research lies at the intersection of many-body dynamics, quantum simulation, quantum control, and applications of machine learning in physics. We are interested in problems of both fundamental nature and immediate applications. We develop approximate analytical methods and design numerical techniques to investigate different problems in quantum dynamics. We collaborate with theory groups and experimental labs to test our theoretical predictions against experiments.

The group consists of 5 postdocs (Patrick Lenggenhager, Suman Mondal, Sourav Nandy, Andrea Solfanelli, and Michael Sonner), 3 PhD students (Giovanni Cemin, Nicolò Beato, and Paul M. Schindler), and 3 shared PhD students (Lauritz Hahn, Noè Salmeron, and James Walkling). The group actively involves undergraduate students to participate in research: bachelor students (Georgi Aleksandrov [Sofia U]), master students (Georgi Aleksandrov [Sofia U], Benoît Fanton [ENS Paris], Teodora Serafimova [Sofia U], Pavel Tashev [Sofia U]), summer interns (Paul Ebert [TU Dresden], Zhanpeng Fu [Shanghai Jiao Tong U], Benjamin Muñoz-Cerro [Stanford], Yubo Shi [Nankai U], Yizhe Sun [Harvard]). Former group members: Dominik Hahn (now postdoc in Oxford), Friederike Metz (now postdoc at EPFL), Pranay Patil (now postdoc at OIST), Mohsen Yarmohammadi (now postdoc at UT Dallas).

Nonequilibrium Dynamics A key challenge in modern quantum simulation and computing is understanding the behavior of excitations generated by external drives used to control these systems. While this problem is complex in general, significant insights can be gained by studying periodically driven (Floquet) systems. These systems occupy an intermediate regime between equilibrium and nonequilibrium dynamics, exhibiting features of both. (i) In collaboration with Ashok Ajoy's experimental group at UC Berkeley, we demonstrated how thermalization can be harnessed to dynamically stabilize structured quantum states. This was achieved in a mesoscopic ensemble of nuclear spins in diamond subjected to strong periodic drives. Building on this work, (ii) we investigated the robustness of spatiotemporal-ordered time-crystalline states against perturbations in the driving protocol. This has direct implications for quantum technologies: by leveraging the sensitivity of prethermal discrete time-crystal (PDTC) order to changes in its order parameter, we developed highly frequency-selective quantum sensors for time-varying (AC) magnetic fields in a strongly driven, dipolar-interacting nuclear spin system. (iii) Recognizing the widespread use of periodic square-wave or pulsed drives in quantum simulation platforms, we developed a framework to analyze Floquet systems in the Walsh basis. This alternative representation, which uses "photon" modes instead of conventional Fourier harmonics, reveals a localized structure of Floquet states under strong kicked or pulsed drives.

Quantum Engineering Over the past decade, periodic drives have become a vital tool for engineering effective Hamiltonians in quantum simulation. These drives allow us to explore behaviors and phenomena that are often inaccessible in conventional materials. A major challenge in quantum simulation today is the realization of spin-liquid states of matter, which can host fractional and non-Abelian anyonic excitations. (i) To address this, we proposed a protocol to implement Kitaev's honeycomb model using periodically-driven ultracold and Rydberg atoms. Our work demonstrated that the periodic drive opens a topological gap in the quasienergy spectrum without coupling the effective Majorana and vortex degrees of freedom. Additionally, we addressed the experimental challenges of probing Majorana fermion physics when only the composite spin degrees of freedom are accessible. In a separate series of works, (ii) we developed a general driving protocol for many-body systems that generates a hierarchy of prethermal regimes, each exhibiting progressively lower symmetry. This approach provides explicit constructions of effective

Hamiltonians and enables the hierarchical imprinting of emergent quasi-conservation laws. The protocol allows quantum simulators to engineer specific symmetries and their associated orders in nonequilibrium matter, facilitating the study of phenomena such as continuous symmetry breaking and the emergence of pseudo-Nambu-Goldstone modes. Finally, (iii) in collaboration with the Ajoy lab, we reported the experimental realization of short-time disorder in a system that exhibits long-time stroboscopic order. Notably, we observed continuous nonequilibrium temporal order, extending beyond the framework of discrete time crystals. This study opens new possibilities for applications leveraging driven quantum matter.

Quantum Control Periodically driven systems have become a powerful tool for engineering the properties of quantum systems and are steadily advancing toward becoming a standard component of the quantum simulation toolbox. However, a key challenge remains: effectively manipulating quantum states dressed by strong periodic drives. The current state-of-the-art in Floquet control relies on the adiabatic tuning of parameters. However, this approach typically requires long protocols, which are often incompatible with the limited coherence times of experimental systems. To enable rapid control of nonequilibrium quantum matter, (i) we extended the concept of variational counterdiabatic driving to nonequilibrium settings, focusing specifically on Floquet systems. Using this approach, we derived a nonperturbative variational principle to construct local approximations to the adiabatic gauge potential for the effective Floquet Hamiltonian. This framework allows for transitionless driving of Floquet eigenstates, even far from the adiabatic regime. Applications include two-level systems, Floquet bands, and interacting periodically driven models. In a follow-up study, (ii) we utilized counterdiabatic driving to establish a connection between Floquet theory and the adiabatic theorem, resulting in a novel geometric framework for periodically driven systems. Interestingly, this work revealed that certain nonequilibrium phenomena without static analogs—such as the π-modes in anomalous Floquet topological insulators or the π-gap pairing in discrete time crystals—may have a geometric origin. As a separate but related research direction, (iv) we investigated control landscape phase transitions (CLPTs), which manifest as abrupt changes in the cost function landscape as a control parameter is varied. These transitions can be identified by nonanalytic points in statistical order parameters. A key example is the emergence of quantum speed limits (QSLs), which delineate the onset of controllability as protocol durations increase. Our work established the foundation for an analytical theory of CLPTs, providing a new lens for understanding and optimizing control in quantum systems.

Reinforcement Learning for Quantum Technology Reinforcement learning (RL) is a branch of machine learning where an agent learns to solve tasks through a feedback loop by interacting with its environment. While RL has demonstrated remarkable success in domains such as achieving superhuman performance in complex games, chip design, and robotics, its applications in quantum technologies remain an area of active exploration. A critical milestone in the development of quantum technologies is achieving control over quantum many-body states. However, the exponential growth of the Hilbert space dimension with the number of qubits presents significant challenges for classical simulation and the design of robust, optimal control protocols. To address this, (i) we introduced a novel framework for efficiently controlling quantum many-body systems using reinforcement learning based on tensor networks. Specifically, we leveraged matrix product states to represent both the quantum physical state and the underlying deep learning architecture, enabling scalable and efficient RL-based control. Model-free approaches are particularly appealing for quantum control tasks, as they do not rely on the often limited accuracy of theoretical models of quantum processors. In this vein, (ii) we developed a continuous-control RL framework to design high-fidelity entangling two-qubit gates for superconducting qubits. Without any prior information about the fixed-frequency, fixed-coupling transmon qubit system, our agent autonomously generated cross-resonance and CNOT gates. The resulting pulse sequences surpassed standard cross-resonance gates in both fidelity and gate duration while maintaining comparable robustness against stochastic unitary noise. An emerging and largely unexplored paradigm in quantum technologies is the use of partial knowledge of quantum states to control multiqubit entanglement. This approach holds potential to address key challenges in quantum state preparation, state compression, quantum control, and quantum complexity. (iii) We developed deep RL methods to construct short disentangling circuits for arbitrary few-qubit states. Ongoing work focuses on scaling these algorithms to larger systems using Clifford gates, opening avenues for broader applications in quantum interactive dynamics.

Collaborations

- Prof. Markus Heyl (Augsburg University, Germany): nonequilibrium dynamics
- Prof. Hongzheng Zhao (Beijing University, China): nonequilibrium dynamics
- Prof. Roderich Moessner (mpi**pks**, Germany): nonequilibrium dynamics
- Prof. Michael Kolodrubetz (UT Dallas, USA): nonequilibrium dynamics
- Prof. Anushya Chandran (Boston University, USA): nonequilibrium dynamics
- Prof. Ashok Ajoy (UC Berkeley, USA): nonequilibrium dynamics, quantum engineering
- Prof. Nathan Goldman (Universite Libre de Bruxelles, Belgium), quantum engineering
- Prof. Monika Aidelsburger (MPQ, Germany): quantum engineering
- Dr. Ricard Alert (mpi**pks**, Germany): nonequilibrium dynamics
- Dr. Markus Schmitt (University of Regensburg, Germany): RL for quantum technology

Research Group: Superconductivity and Magnetic Correlations
(since January 2023, Head: Dr. Alexander Wietek)

The "*Superconductivity and Magnetic Correlations (SuMaC)*" group was started in January 2023. Our key objectives are to discover and understand strongly correlated phases of matter in superconducting and magnetic compounds. This ranges from puzzles posed in frustrated magnets, such as the quest for identifying quantum spin liquids, to understanding unconventional forms of superconductivity as found in high-temperature superconductors, kagome metals, and moiré materials. The fundamental models capturing essential aspects of these phenomena such as the Hubbard model are also studied in collaboration with experimental quantum simulation groups. A strong focus of our work also lies in the development of modern algorithms for solving the quantum many-body problem, such as tensor network algorithms. The group is funded by the Emmy-Noether program of the German Research Foundation (DFG) and consists of four PhD students (Luke Staszewski, Hannes Karlsson, Rafael Soares, Paul Ebert) and two PostDocs (Aritra Sinha, Martin Ulaga).

Strongly correlated superconductors Superconductivity ranks among the most fascinating phenomena in condensed matter physics. A focus of our group lies in unraveling the nature of superconducting states occurring in microscopic models of superconductivity. Recently, we have found that charge density waves can coexist with superconductors, forming supersolid states, in simple variants of the Hubbard and t-J model. We found that this coexistence can lead to a so-called "fragmentation" of the condensate, where more than one Cooper-pair wave function is macroscopically occupied. Moreover, we are currently working on a precise definition of Cooper-pair localization length and study this across the BCS-BEC crossover in the attractive Hubbard model in a magnetic field hosting a Fulde–Ferrell–Larkin–Ovchinnikov phase. Our future aim is to develop a thorough understanding of novel superconducting states found in kagome metals, nickelate superconductors, and moiré compounds based on microscopic descriptions of these recently discovered compounds.

Frustrated magnetism Frustrated magnets are potential hosts of exotic states of matter. One focus of our group was the prediction of spectroscopic experiments at finite temperatures. Together with the former postdoc Zhenjiu Wang, we recently developed a new finite-temperature tensor network algorithm employing complex time correlation functions and applied this to the anomalous thermal broadening of the neutron scattering intensity of $SrCu_2(BO_3)_2$ and associated Shastry-Sutherland model. In another recent collaboration with the experimental group of Prof. Elena Gati, the PhD student Rafael Soarez and I are investigating elastocaloric effects in $SrCu_2(BO_3)_2$. Elastocaloric experiments are novel and precise probes of quantum phase transitions and serve as a motivation for us to develop the numerical methods to capture these experiments. On a theoretical side, we have performed detailed investigations of the excitation spectrum of the putative Dirac spin liquid stabilized on the triangular lattice antiferromagnet relevant to recent delafossite compounds. A future goal of our group is to understand dynamical properties of quantum spin liquids relevant to their experimental detection.

Physics of the pseudogap regime We investigate how the superconducting or other strongly correlated phases such as stripes emerge at low temperatures. In particular, the so-called pseudogap and strange metal regimes in the two-dimensional Hubbard model exhibit several fascinating features not fully understood so far. Using novel finite-temperature tensor network techniques we are now in the position to perform accurate microscopic simulations in these temperature ranges. We discovered that above the transition to a stripe-ordered ground state, doped holes in an antiferromagnet form extended

clusters of lower hole density with a statistical distribution of sizes. We named this scenario "forestalled phase separation" as it is strongly reminiscent of thermodynamic phase separation into Mott insulating and hole-rich regions. In collaboration with the experimental group of Prof. Immanuel Bloch, we have further investigated the magnetic properties of the onset of the pseudogap regime. We discovered a doping-independent scaling of the spin correlation length with temperature. The characteristic energy scale extracted from experimental measurements agrees closely with an estimate of the pseudogap onset temperature T^* determined numerically using minimally entangled thermal typical states. Our joint study also demonstrated that temperatures in strongly correlated regimes can now be accessed in experiments where accurate comparisons with computational methods are possible. Our future aim is to understand how the observed clustering of charge carriers affects transport and spectroscopic properties in the pseudogap and strange metal regime.

Dynamics of the strongly correlated electrons Ultra-cold atom experiments provide us with new means of investigating the dynamical properties of strongly correlated systems. Feshbach spectroscopy refers to driving an interacting system by modulating an applied magnetic field and, thereby, modulating the interaction strength. In collaboration with the experimental group of Prof. Martin Zwierlein, we are investigating the response of the attractive Hubbard model with respect to such a modulation. Comparing results from linear response and exact numerical time evolution reveals novel insights into the physics of the pairing mechanism. Together with the PhD student Luke Staszewski, we investigated the physics of a quench in the chemical potential in the two-dimensional t-J model. The dynamical behavior is found to range from ballistic transport for stripes to complete dynamical freezing in the phase-separating regime.

Theoretical collaborations:

- Paul McClarty (Université Paris-Saclay, CEA Saclay, France)
- Andreas Honecker (Cergy Paris Université, Cergy-Pontoise, France)
- Andreas Läuchli (Paul Scherrer Institute, Villigen, Switzerland)
- Sylvain Capponi (Laboratoire de Physique Théorique, Université de Toulouse, CNRS, UPS, Toulouse, France)
- Antoine Georges (Flatiron Institute, New York, USA, and Collége de France, Paris, France)
- Matthew Fishman (Flatiron Institute, New York, USA)
- Zhenjiu Wang (Lanzhou University, Lanzhou, China)
- Niccolo Baldelli (ICFO, Barcelona, Spain)

Experimental collaborations:

- Immanuel Bloch (Max-Planck-Institut für Quantenoptik, Garching, Germany)
- Thomas Chalopin (Université Paris-Saclay, Palaiseau, France)
- Timon Hilker (University of Strathclyde, Glasgow, United Kingdom)
- Martin Zwierlein (Massachusetts Institute of Technology, Cambridge, Massachusetts, USA)
- Elena Gati (Max Planck Institute for Chemical Physics of Solids, Dresden, Germany)

Awards of people in the group:

- Aritra Sinha: Alexander von Humboldt Research Fellowship

Division: Finite Systems
(Head: Prof. Jan Michael Rost)

The department *Finite Systems* studies finite microscopic systems and their interaction with an environment in the extreme regimes of ultracold and ultrafast dynamics and from a fundamental quantum aspect. Finiteness can refer to a finite number of particles, e.g., atoms or molecules, to geometric restrictions in real space or in abstract mathematical spaces. The environment can consist of similar entities as the atom or molecule under consideration (e.g., clusters, quantum aggregates, ultracold gases). Secondly, light from intense pulses or in cavities provides another kind of environment. Thirdly, noise creates an important class of environment, also studied at mpi**pks** outside the *Finite Systems* department in various contexts, from cavities over chaotic dynamics to biological systems.

The research group *Finite Systems* within the department has presently three thrusts: The first one concerns fundamental time-dependent mechanisms in light-matter coupling. Here, we concentrate on short pulses relating the fields of attosecond and time-dependent X-ray science and in general strong field physics (project leader *Ulf Saalmann*). The second focus lies on ultracold finite systems where we study quantum droplets (project leader *Panos Giannakeas*) and ultracold Rydberg excitations in structured environments together with the groups of *Matthew Eiles* and *Alexander Eisfeld*, whose experience with polarons and exciton dynamics in traditional quantum aggregates, respectively, is very valuable in the context of ultracold Rydberg complexes. Thirdly, we investigate forms and properties of system environmental coupling from a more fundamental perspective. The affiliated Research Group *Strongly Correlated Light-Matter Systems*, headed by *Francesco Piazza*, was interested in systems coupled to structured environments formed by cavities and provided a fruitful bridge to the condensed matter department.

Research topics

Many-body phenomena with a Rydberg electron. Anderson localization and topological properties are typical remnants of many-body dynamics. We are interested in their counterparts involving Rydberg excitation. The latter can lead indeed to Anderson localization of the Rydberg electron which exhibits a thermodynamic limit when approaching the ionization threshold while encompassing in its huge orbital volume many atoms of a gas at random positions. We also are interested in coherent properties of ultracold quantum droplets. Doping a helium droplet with a suitable ion, we have discovered that the coexistence of a crystal like structure and a superfluid can give rise to supersolidity, which can be eventually probed by a Rydberg electron. To this end we have developed a semiclassical/meanfield hybrid method which can handle orders of magnitude larger particle numbers than full Quantum Monte Carlo calculations.

Time-dependent few photon dynamics. Combining time-dependent properties of a classical laser pulse (such as chirp and envelope) with few photon quantum processes for the direct interaction with matter, as is the case for XUV photons, offers interesting perspectives, in particular since the control of such pulses is now possible at FEL sources, e.g., in Trieste. We have found that two photon processes from an attosecond pulse can lead to an uncoventional "zero-energy" photo effect, where the photoelectron peak remains at the same energy when varying the photon's wavelength, but shifts in energy when the pulse length is changed. Fano resonances controlled by attosecond pulses as well as the Kapitza-Dirac effect in the time domain are further realizations of such dynamics.

Machine learning beyond a numerical tool. Presently, we have three projects which apply machine learning.(i) With a Generative Avdversarial Network (GAN) we reconstruct from single shot diffractive 2D images directly the 3D image of the target molecule in reciprocal space, without sorting the 2D images. (ii) We obtain an effective Hamilton matrix without knowing details of the underlying system from feeding a 2D spectrum to a Deep Neural Network trainded on data of a large variety of random systems. The hamiltonian obtained can be used to calculate different properties of the system beyond its spectrum. (iii) Using the difference of the output from a linear and a non-linear decoder, we can determine the "excess entropy" which is a measure of the complexity underlying an irregular looking time series.

Symmetries in open systems and emergent relations when separating system and environment. Here, we have developed a semiclassical concept to understand the prerequisites for long-time non-stationary dynamics, namely symmetries that permit an isolation from the environment leading to decoherence free subspaces. From a different perspective, we want to see how in a fully quantal setting time and temperature emerge from a global entangled eigenstate state through the separation of system and environment.

Perspectives for the future

We will continue to work along the two strongholds of the department, ultracold and ultrafast dynamics, in close collaboration among the senior members of the department. Integration of AI into our research beyond using it as a numerical tool will be re-enforced by exploiting the very well developed AI-based imaging recognition capabilities for processing and classifying large Hamilton matrices as square arrays of pixels. Furthermore, of risky and truly exploratory nature will be the question if the recently discovered expanded neural network of inhibitory neurons in the human cortex, controlling the excitatory neuron network, can be understood from adversarial bipartite tensor networks which we will formulate in Dresden

and implement in a minimalistic way on an experimental quantum processor in Mainz to take systematically realistic losses of coherence and entanglement into account, before comparing to measured properties of the brain networks. A quantum origin could explain the extraordinary efficiency of the brain's network architecture. The project will unfold in a collaboration between Moritz Helmstaedter (director MPI for brain research, Frankfurt), Julijana Gjorgjieva (chair for theoretical neuroscience, TU Munich), Ferdinand Schmidt-Kaler (QUANTUM project, Uni Mainz) and the groups of *Marin Bukov* and *Jan Michael Rost* at mpi**pks**.

Collaborations

- Prof. H.-J. Wörner (ETH Zürich, Switzerland) on attosecond resolved observables,
- Prof. C. H. Greene (Purdue University, USA) on ultracold non-adiabatic effects,
- Prof. L. Khaykovich (Bar-Ilan Univ., Israel) on non-adiabatic ultracold gas experiments,
- Prof. N. Berrah, (U. Mass., USA) on XFEL induced collective electron effects,
- Prof. T. Pfeifer (MPI for Nuclear Physics, Heidelberg) regarding ionization in XUV pulses,
- Prof. K. Singh (IISER, Mohali, India) on attosecond ionization,
- Prof. R. Dörner (Uni Frankfurt) on electron-photon scattering,
- Prof. S. Wüster (IISER Bhopal, India) on electron transport in Rydberg aggregates,
- Prof. F. Stienkemeier (Uni Freiburg) on XUV-FEL induced dynamics in atoms,
- Prof. T. Pohl (TU Wien, Austria) on supersolidity

Local collaborations

With Prof. F. Großmann, TU Dresden, on *semiclassical light matter interaction*.

Research Group: Quantum Aggregates
(Head: Dr. Alexander Eisfeld)

The group was established in October 2012. Since 2019, the group leader Alexander Eisfeld is funded via a Heisenberg fellowship of the German research foundation (DFG). From Jan 2023 to Oct 2024 he had a temporary professorship at the University of Potsdam. Since April 2024 he has a permanent position at the TU Dresden.

Currently the group at the mpi**pks** consists of three PhD students (Sidharta Nayak, Juan Moreno and Aritra Mishra) and two postdoctoral guest scientists (Grace Hsiao-Han Chuang and Ritesh Pant). During the evaluation period the group hosted another postdoctoral guest scientist (Abhijit Pendse).

The main focus of our research is the emergence of collective quantum effects in mesoscopic assemblies of atoms and molecules (aggregates), where the individual atoms/molecules interact via long range forces. In particular we are interested in the interplay between electronic and nuclear dynamics and its influence on optical and transport properties. Some concrete examples are given below:

Molecular aggregates on dielectric surfaces We consider various situations in collaboration with experimental groups: molecules are deposited either under ultra-high vaccum (group of Prof. Sokolowski, Bonn), in solution (groups of Prof. Hauer, TUM, and Dr. Mertens, Lancaster) or on rare earth clusters (group of Prof. Stienkemeier, Freiburg). Regarding molecules on rare earth clusters, our main interest is the influence of the cluster material on the lifetime and quantum yield of acene molecules, from which we draw conclusions about non-radiative channels such as singlet fission. For regular monolayers on surfaces we have indications that electronic excitation is coherently shared by hundreds of molecules. We investigate the use of metallic tip based near-field spectroscopy to gain access to these eigenstates and to map out their wavefunctions. We achieve this by using neuronal networks trained on calculated position dependent near field spectra. At present, we are exploring the information that pump-probe spectroscopy can provide about dephasing and relaxation pathways to gain further insight into the interaction of the molecules with the surface. Recently, we have also become interested in the topological properties of regular molecular aggregates on surfaces, with individual molecules that exhibit degenerate transitions.

Stochastic Schrödinger equations for open quantum system dynamics Open quantum system approaches are widely used in the description of physical, chemical and biological systems to handle the coupling of electronic degrees of freedom to vibrations. A structured vibrational environment consisting of internal molecular modes and solvent modes leads to long-lasting non-Markovian dynamics, which

makes numerical simulations quite demanding. Instead of using a master equation, we tackle the problem by solving a stochastic Schrödinger equation of the diffusion type which gives the exact reduced density operator in the electronic subspace. In collaboration with Prof. Strunz from the TU Dresden, we have derived an exact hierarchy of coupled stochastic equations (HOPS) for the propagation of pure states. This hierarchy provides a numerically exact and efficient method, since one can use the localization properties of individual trajectories. We have succeeded in extending the formulation to the calculations higher order time-correlation functions to handle multidimensional femto-second spectroscopy. In the last two years we have applied this method to large photosynthetic light harvesting systems and self-assembled molecular aggregates in solution.

Interacting Rydberg assemblies Atoms excited to high principal quantum numbers (so-called Rydberg atoms) can interact strongly with other Rydberg atoms or ground state atoms at micrometer distances. We investigate properties and applications of both types of interaction. The interaction between Rydberg atoms with different angular momenta can lead to collective states akin to the exciton states of the molecular aggregates mentioned above. These states can be created and probed via microwave pulses. The ability to place atoms in nearly arbitrary arrangements and strongly tune their interactions by selecting specific Rydberg states allows us to study various types of disorder in a controlled way. While for this interaction, the extent of the Rydberg wavefunction is smaller than the Rydberg-Rydberg separation, the other type of setup requires the ground state atoms to be within the Rydberg wavefunction. In both cases, a particular focus is on coupling to vibrational modes provided, for example by the external trapping potential.

Collaborations:

- Dr. Eiles (mpi**pks**): Rydberg atoms.
- Prof. El-Ganainy (Michigan Tech, USA): Non-linear photonics.
- Prof. Hauer (TUM): Spectroscopy of organic dye aggregates.
- Prof. Mertens (Lancester,UK): Molecules on surfaces.
- Dr. Mostame (IBM, New York): Digital quantum simulator.
- Prof. Rost (mpi**pks**): Rydberg composites.
- Prof. Saalmann (mpi**pks**): Transition currents.
- Prof. Sokolowski (Uni Bonn, Germany): PTCDA monolayers on dielectric surfaces, superradiance.
- Prof. Stienkemeier (Uni Freiburg, Germany): Phase-modulated spectroscopy, molecules on clusters.
- Prof. Strunz (TU Dresden, Germany): Stochastic Schrödinger equations.
- Prof. Wüster (IISER Bhopal): Rydberg aggregates in Bose Einstein condensates.

Research Group: Strongly Correlated Light-Matter Systems
(until September 2024, Head: Dr. Francesco Piazza)

The research group "Strongly-Correlated Light-Matter Systems" was part of the institute between March 2017 and October 2024. The group leader Francesco Piazza has moved to the University of Augsburg in October 2023, afterwards running the group for one more year with a double affiliation. Since the last scientific report, two students completed their PhD: Christian Johansen (now a PostDoc at the University of Trento) and Mariano Bonifacio (moved to industry). Moreover, the postdoc Tomasz Wasak became a faculty at the University of Torun, and the postdoc Johannes Lang moved on for a second postdoc at the Unversity of Cologne. Three more members also joined: Igor Gianardi (PhD student since 2023), Michele Pini (Postdoc since 2022, moved to Augsburg in 2024), and Mursalin Islam (Postdoc since 2023, will move to Augsburg in 2025).

General topic. Our research area lies at the boundary between condensed matter physics and quantum optics, and deals with quantum many-body open systems.

Systems. Our investigations are strongly related to ongoing experiments in hybrid light-matter systems which implement variations of Quantum Electrodynamics (QED) in the strong-coupling regime. So far the focus has been mainly on ultracold atoms coupled to light in optical waveguides or cavities. More recently, the scope has extended to include correlated electrons in solid state.

Approach. We develop non-equilibrium field-theoretical methods, tailored for the study of many-body phenomena in the above open quantum systems. These approaches are novel in the context of quantum optics and non-trivially extend methods typically used in condensed matter.

Goals. We are interested in fundamental theoretical problems in many-body physics like collective phenomena and non-equilibrium phases. However, since our techniques are quantitatively reliable, we also concretely investigate hybrid light-matter devices for applications in the control of material properties as well as quantum nonlinear optics and metrology.

Merging approaches from condensed-matter and quantum-optics theory is a necessary step for the description of the many-body physics arising in QED within correlated quantum materials. Let me provide three examples where this merger between approaches eventually led to a merger between paradigms from condensed-matter- and quantum-optics-theory.

Merging Superradiance with Non-Fermi-Liquids. In quantum optics, superradiance is a paradigmatic effect of collective light scattering from an ensemble of particles, which can even manifest in the ground-state as a phase transition across which macroscopic order in the material appears in concomitance with a photon condensate. In a recent work [1], we have shown that the critical photon fluctuations at the superradiant phase transition can induce non-Fermi-Liquid behavior in an electronic system – a paradigmatic effect in condensed matter whereby strong collective fluctuations lead to the destruction of quasi-particles.

Merging the Quantum-Zeno-Effect with Polarons. In this work [2], the Zeno effect from quantum measurement theory meets the quantum impurity problem at the border between few- and many-body physics. The resulting novel type of polaron quasiparticle we predict, and the underlying modification of in-medium scattering in presence of strong loss, constitute an important insight and a systematic step towards understanding the interplay between strong measurement and intrinsic many-body correlations.

Merging Nonclassical Light with Superconductivity. Can the pairing between electrons (and in turn superconductivity) be influenced by preparing the quantum state of the "glue"? This question becomes especially relevant in cavity-quantum materials, where the glue can be provided by photons instead of phonons. The former can be much more easily pulled away from the thermal state in equilibrium with the electrons, and even prepared in a non-classical state using methods from quantum optics. In these recent works [3, 4], we have shown that such photon-glue-state preparation can be used to enhance and even qualitatively modify pairing and superconductivity.

[1] P. Rao and F. Piazza, Phys. Rev. Lett. **130** (2023) 083603.
[2] T. Wasak, R.Schmidt, and F. Piazza, Phys. Rev. Res. **3** (2021) 013086.
[3] A. Chakraborty and F. Piazza, Phys. Rev. Lett. **127** (2021) 177002.
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Research Group: Correlations and Transport in Rydberg Matter
(Head: Dr. Matthew Eiles)

The group *Correlations and transport in Rydberg matter* was established in January 2021 and currently consists of three PhD students (Aileen Durst, Neethu Abraham, and Milena Simić) and two postdoctoral guest scientists (Taha Alper Yoğurt and Homar Rivera-Rodríguez). During the evaluation period, three other postdocs were members of the group - Viktor Ivády (now assistant professor at Eötvös Loránd University, Budapest), Frederic Hummel (now quantum theorist at Atom Computing), and Črt Lozej (now employed at d-fine). Additionally, we hosted a master's student from the University of Warsaw, Agata Wojciechowska (May 2021), and Dr. Mykhalo Khoma from NASU (from May 2024).

Our research focuses on highly excited Rydberg atoms and the phenomena which emerge as a result of their exaggerated length, energy, and time scales. Two primary motivations guide us. First, we want to understand and interrogate dynamical processes in and fundamental properties of microscopic systems. Rydberg states are spatially extended and probe their local environment through their interactions with it, providing a versatile and experimentally powerful lens with which to investigate disparate physical phenomena ranging from few-body systems to many-particle aggregates. Second, we want to explore novel composite systems which become apparent or can be created by interfacing excited Rydberg atoms with an environment, for example one composed of other Rydberg atoms, ions, or ground-state atoms. In *Rydberg matter* of this kind, Rydberg excitation magnifies the interactions between these components and allows for the environment to exploit the vast size and degeneracy of Rydberg states.

Below is an overview of our recent research activities.

Long-range Rydberg molecules: Several varieties of long-range Rydberg molecules characterized by remarkably large bond lengths and fragile binding mechanisms have been observed in ultracold gases.

- *Precise determination of electronic potentials:* Molecules composed of a Rydberg atom and a ground-state atom rely on the spatial overlap between the Rydberg electron and the ground-state atom for their binding mechanism. This leads to unusual oscillatory potentials, which in the standard approach are calculated utilizing contact pseudopotentials expanded into a basis of electronic orbitals. Although this method yields a qualitative description from which key predictions can be made, it is known to not be convergent, hindering spectroscopic assignment of observed vibrational levels. We have reformulated the theory to exploit the Coulomb Green's function to circumvent this convergence issue. In collaboration with experimentalists in Kaiserslautern, Ulm, and Durham, we have employed this method to interpret complex experimental vibrational spectra and to extract fundamental atomic scattering parameters which are otherwise energetically inaccessible in collision experiments.
- *Vibronic coupling and non-adiabatic dynamics:* The interplay between these oscillatory potential energy curves and the energy level structure of the individual atomic constituents results in many narrow avoided crossings. Near these, beyond-Born-Oppenheimer effects can manifest. We have explored these effects using a combination of large-scale numerical calculations to solve the full vibronic coupled-channel equations for both bound and scattering states and simpler qualitative models to provide physical insight. One hallmark of Rydberg molecules in alkaline elements is a fragility borne out of resonant electron-atom scattering which can destabilize the whole molecule. Counterintuitively, we have found that non-adiabatic coupling can counteract this, and have identified that this occurs due to the nodal structure of the Rydberg wave function.
- *Dynamics and structure of molecular Rydberg ions:* The multipolar interaction between a Rydberg atom and a cation is attractive at long-range and steeply repulsive at short-range; when these forces are in equilibrium a long-range molecular ion forms. We have studied the predissociation of this molecule using multichannel scattering to calculate the decay rate, which turns out to be remarkably sensitive to the number of decay channels. This appears to result from an interference mechanism, which we are developing a semiclassical framework to interpret. Further exploiting the possibility of interactions in these systems to delicately balance one another, we have also predicted that triatomic dications - two ions bound to a Rydberg atom - are also (meta)stable and can be experimentally excited.

Rydberg atoms and molecules in optical tweezer arrays: Atoms trapped in optical tweezers arrays have become a mainstay of ultracold atom laboratories. By arranging these atoms into desired geometries and promoting them to Rydberg states, their long-range interactions in the confined geometry of the tweezer array allow for quantum simulation. We investigate the scenario with only a single Rydberg atom, where it is the Rydberg electron which mediates the long-range interaction between the Rydberg atom and its neighboring atoms rather than the usual dipole-dipole interactions between Rydberg atoms.

- *Rydberg composites and quantum simulation in a dense tweezer array:* When a Rydberg atom is interfaced with an array of many ground-state atoms, the latter structure the otherwise highly degenerate spectrum of the Rydberg atom and sculpt its electronic wave function. We have recast the *Rydberg composite* Hamiltonian into a tight-binding form, highlighting a deep connection between the excited states of atomic spectra and foundational solid-state models. With this reformulation we demonstrate how the hydrogenic properties inherited by a Rydberg atom enable a thermodynamic limit, and studied Anderson localization of the Rydberg electron. The interplay between the effectively zero-ranged interaction of the Rydberg electron with the ground-state atoms and the infinite-ranged Coulomb interaction with the ionic core lends a remarkable degree of tunability to the system, which we exploit to design Rydberg composites such that the Rydberg electron exists in a topological edge state protected by a chiral symmetry (as in the SSH model) or an inversion symmetry (as in a collection of coupled trimer subsystems).
- *Molecular physics in small tweezer arrays:* We have studied heteronuclear Rydberg molecule formation in by optical tweezers in collaboration with the experimental group of Simon Cornish. By using two different tweezer wavelengths, they have produced Rydberg molecules using Rydberg Rb and ground-state Cs both within the same tweezer trap and in tweezers nearly 300 nanometers

apart. This work paves the way for possible future explorations of mediated transfer of vibrational excitation between atoms in tweezers or the control of the Rydberg electron by tweezer manipulation.

Impurities in ultracold gases. We investigate the absorption spectrum of a Rydberg impurity immersed in and interacting with an ideal Bose-Einstein condensate. Here, the impurity-bath interaction can greatly exceed the mean interparticle distance; this discrepancy in length scales challenges the assumptions underlying the universal aspects of impurity atoms in dilute bosonic environments. Our exploration thus offers insights into the interplay between interaction range, density, and many-body behavior in impurity systems, which we have supplemented with an exploration of other impurity species. Expanding on this, we are engaged in the development of additional numerical treatments of long-range impurities including the coherent state Ansatz and a perturbative Gross-Pitaevskii treatment. These allow us to include the interactions between bath particles and finite polaron momentum, and in turn compute their quasiparticle weight and effective mass, permitting a more quantitative treatment of the phenomenology of long-range impurities.

Quantum scarring, localization, and chaos. The same properties which make Rydberg atoms in an impurity environment fascinating can be found in many other systems, for example in quantum dots, electrons moving in magnetic fields, and semiconductor excitons. By adapting our Rydberg toolkit to these systems, we investigate the underlying connections between quantum scarring induced by disorder, quantum chaos and semiclassical dynamics, and Anderson localization.

Collaborations with experimentalists

- Prof. Simon Cornish (Durham University): Rydberg molecules in optical tweezer arrays.
- Dr. Stephan Dürr (MPQ, Garching): Photon storage and retrieval.
- Prof. Johannes Hecker-Denschlag (Ulm University): Rydberg molecule formation and dynamics.
- Prof. Sebastian Hofferberth (University of Bonn): Rydberg molecule spectroscopy of ytterbium.
- Prof. Herwig Ott (RPTU Kaiserslautern-Landau): Precision Rydberg molecule spectroscopy.

Collaborations with theorists

- Dr. Alex Eisfeld (mpi**pks**): Rydberg aggregates and Rydberg composites.
- Dr. Panagiotis Giannakeas (mpi**pks**): Few-body physics.
- Prof. Chris Greene (Purdue University): Green's function methods.
- Prof. Seth Rittenhouse (United States Naval Academy): Rydberg polarons.
- Prof. Jan-Michael Rost (mpi**pks**): Rydberg composites and long-range Rydberg molecules.
- Prof. Hossein Sadeghpour (Harvard, USA): Rydberg polarons.
- Prof. Peter Schmelcher (University of Hamburg): Non-adiabatic dynamics and exotic molecules.
- Prof. Michał Tomza (University of Warsaw): Rydberg molecules composed of complex atoms.

Division: Biological Physics
(Head: Prof. Frank Jülicher)

Living matter is an inherently dynamic and highly organized form of condensed matter that is maintained away from thermodynamic equilibrium. The division *Biological Physics* develops theoretical approaches to study the spatiotemporal organization of living matter at scales ranging from molecules to cells and tissues. This research is done in tight interaction with quantitative experiments and in interdisciplinary collaborations at the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) and the Center for Systems Biology Dresden (CSBD). The study of living matter as a physical system is based on an integration of statistical physics, soft matter physics and nonlinear dynamics. A key goal is to identify fundamental principles that underlie the self-organization of complex cellular processes such as cell division, intracellular transport, the spatial and temporal organization of organelles as well as the collective behaviors of many cells. A key example is to study how complex morphologies and patterns emerge when an organism develops from a fertilized egg. Living matter is fundamentally active and driven far from thermodynamic equilibrium by a supply of free energy via metabolic processes. It exhibits significant stochasticity while operating robustly even when perturbed. The study of living matter poses

many challenges related to its enormous complexity and its nonequilibrium character. However important breakthroughs have been made in recent years. A key example is the insight that biological structures emerge from the self-organization of active mechano-chemical, sometimes mechano-electro-chemical processes. A second example is the study of biological condensates, which can be understood as phase separated droplets that organize and position active biochemical processes in the cell.

In our group, we investigate specific biological processes in close collaboration with experiments to reveal underlying physical principles. We also develop general theoretical approaches to the complex dynamics of soft active matter, the role of fluctuations and the emergence of patterns and shapes.

Recent examples of our research include:

Formation of Liquid Shells in Active Droplet Systems. Liquid mixtures can undergo phase separation and demixing. Such mixtures can also host different chemical processes. We investigate the physics of phase separating systems that undergo chemical reactions. Recently, we showed that liquid shells can form as stable structures in active emulsions. These structures can be understood theoretically and have been observed experimentally.

Dynamic instability of intracellular condensates. In collaboration with the group of Stephan Grill we have shown that the activation of the acto-myosin cortex involves the formation of large numbers of dynamic condensates. These condensates are chemically active. They first grow and subsequently shrink and disassemble via a dynamic instability. This phenomenon can be understood by a nonlinear dynamic system that involves homoclinic orbits. We find that condensate dynamics follow mass action kinetics that governs both composition and size. This dynamic instability could allow the cell to control autocatalytic filament assembly in the cell, which otherwise would be inherently unstable.

Wetting phenomena in cell biology. Epithelia are two dimensional tissues where cells are closely packed to form a confluent surface. The confluence of the tissue is enabled by tight cellular junctions between cells. In collaboration with the group of Alf Honigmann, we have recently shown that tight junctions form by a wetting phenomenon. Here, proteins condense on the membrane interface to form a fluid protein layer. This material provides a scaffold for subsequent junctional assembly. A simple model of surface condensation can account for the observed kinetics of junction elongation.

Topological morphogenesis. Epithelia can form surfaces of different topologies. In collaboration with Elly Tanaka, we have investigated how the topology of neuroepithelial organoids is changing during morphogenesis. We revealed that topology changes via trans and cis fusion events of tissue surfaces, with rates depending on levels of signaling molecules. Untreated organoids formed closed surfaces with a topological genus that increased with time.

Geometry sensing and cell rotations. Cell division is the result of active processes in the cell cytoskeleton such as the self-organization of the mitotic spindle and the contractility of the cell cortex. A key biological question is what determines the orientation of the cell division axis. In 1884 Oscar Hertwig suggested that cells divide along their long axis. In collaboration with Stephan Grill, we studied the role of cellular geometry in rotations that orient the spindle during division. We showed that cortical contractility generates a torque which can lead to rapid spindle rotation inside the cell. These rotations orient the spindle along the long axis and determine the division axis.

Physics of odd visco-elastic materials. Active chiral matter can exhibit unconventional odd material properties. An example is odd elasticity, which can perform work under quasistatic cycles. We investigated odd material properties in visco-elastic systems and revealed that odd visco-elasticity can exist in passive systems. We show that odd properties are revealed in the motion of probe particles. In particular in active regimes, partice motion can become unstable and generate spontaneous motion.

Integration in the Dresden scientific environment

Dresden has developed a flourishing scientific environment at the interface of physics and biology. Most important is a longstanding joint research program of mpi**pks** and the MPI-CBG. We are closely collaborating with research groups at MPI-CBG to bring physical approaches to biology for the study of living matter. Our department is also linked to the International Max-Planck Research School for Cell, Developmental and Systems Biology, managed by the MPI-CBG. This permits PhD students to be fully integrated both with Physics and Biology.

We are tightly integrated in the Center for Systems Biology Dresden (CSBD), which is jointly operated by the MPI-CBG and the mpi**pks** in partnership with the Technical University Dresden (TUD). The CSBD

provides a hub that facilitates the interaction of theoretical physics, mathematics and computer science with cell and developmental biology. It stimulates collaborations and opens new research directions. It also brings us in proximity to the experiments next door to the new CSBD building.

An important partner in our research is the Cluster of Excellence Physics of Life (PoL) at TU Dresden. The cluster was established in 2019 and has developed rapidly. Several new research groups with high international visibility were recently attracted to PoL. The PoL Cluster of Excellence provides a stimulating research environment, bringing new exciting research directions to Dresden.

Collaborations

- Max Planck Institute of Molecular Cell Biology and Genetics, Dresden
  - Stephan Grill, Anthony Hyman, Ivo Sbalzarini and Christoph Zechner on cell physics.
  - Anne Grapin-Botton, Nathalie Dye, Stephan Grill, Carl Modes on the dynamic organization of tissues.
- Cluster of Excellence, Physics of Life, TU Dresden
  - Alf Honigmann on condensate wetting in the formation of cell junctions.
  - Jan Brugués on active cellular matter.
  - Otger Campàs on the biophysics of tissues in developing organisms.
  - Rita Mateus on tissue regeneration.
- Institut Curie, Paris
  - Jacques Prost on on active matter and cell and tissue physics.
  - Pascal Martin on active cellular processes.
- Collège de France, Paris
  - Jean-Francois Joanny on the self organization of active matter and the physics of metabolic processes.
- Max Planck Institute for Multidisciplinary Sciences, Göttingen
  - Jochen Rink on branching morphogenesis and organism scaling.
- Universität Augsburg
  - Christoph Weber on chemically active droplets.
- University of Geneva
  - Marcos González-Gaitán on tissue scaling and growth control.
- Leiden University
  - Louise Jawerth on material properties of condensates.
- Institute of Molecular Pathology, Vienna
  - Elly Tanaka on topological morphogenesis.

Research Group: Nonlinear Time Series Analysis
(Head: Dr. Holger Kantz)

The world surrounding us is in permanent motion, most of which is irregular in detail despite regularities on coarser scales. A good example is the weather, which is subject to clear and easily understandable seasonality, but which poses severe challenges when we want to predict the irregular deviations from the annual cycle. The "fuel" for such fluctuations is transport through a system, usually energy or mass, which means that such systems are open or driven. The research of our group is devoted to the characterisation, modelling, understanding, and prediction of fluctuations in open classical systems, and using this methodology to study specific systems and phenomena.

Our research is in non-equilibrium statistical mechanics, low- and high-dimensional dynamical systems, and nonlinear stochastic processes driven by Gaussian and non-Gaussian noises. These are fields where fluctuations play a dominant role and which are closely related to each other. As example, the understanding and characterisation of deterministic chaotic motion has benefited in the past from mapping it to stochastic processes with short or even long range memory. A particular field of application is the

Earth's atmosphere and climate, a very complex driven dynamical system where predictions of short and long time spans are of the utmost general interest. One issue that is repeatedly raised in connection with climate change is the suspected change of the frequency and intensity of extreme weather events. Analysing these poses particular challenges due to their rarity and the lack of a robust observational basis.

Long range temporal correlations We have continued our long-standing work on the statistical analysis and consequences of long-range temporal correlations (LRC) in data and in model processes. In the past three years, our PhD student Johannes Kassel has made significant progress in using such correlations to improve predictions. While in the past the focus was on the detrimental effects due to redundancy in data and reduced information content, our PhD student Johannes Kassel was able to extract useful information about the future from the long-range correlated past. For details see Sec.2.

Another extension of previous work was achieved in a larger collaboration with major contributions from our Post-doc Samudrajit Thapa. We introduced a new model process with time-varying Hurst exponent, along with a statistical inference method and change point detection. In a first explorative study we observed such changes in atmospheric temperature data around the globe. While we understood the consequences of these changes on the accuracy of the determination of the warming trend, we are still unaware of the physical mechanism that causes them.

Multiplicative noise In the theory of stochastic processes, noise is called multiplicative if its amplitude depends on the state variable. Our PhD student Ewan Phillips identified a previously unexplored effect: multiplicative noise can strongly enhance the probability of the trajectory being at the position in phase space where the noise amplitude is minimal. This finding is particularly relevant for understanding the synchronisation of flagella in unicellular organisms.

ENSO, heat waves, flood risks, global warming Within the European ITN CAFE *Climate advanced forecasting of sub-seasonal extremes*, our PhD student Xinia Hu studied the predictability of the El Niño Southern Oscillation (ENSO) phenomenon as well as related flood risk in South America and in Africa. Emmanuel Rouges tested the usefulness of atmospheric circulation patterns as large-scale and long-lived objects for their impact on predictions of European heat waves in another sub-project. The ITN ended in 2023, and both PhD students successfully defended their PhDs within the expected time. We continue to study atmospheric phenomena in one master's thesis, where we confront the prediction of ENSO by reservoir computing with classical, physics based prediction schemes. Another Master's thesis focuses on the correlation of temperature and precipitation. We are examining the relevance of the Clausius-Clapeyron relation for the water vapour saturation pressure as a function of temperature for extreme precipitation. While in theory the capacity of the atmosphere to absorb (and hence carry) humidity increases by roughly 7% for each 1K temperature increase, many processes might amplify or mitigate this effect in reality. In another project our post-doc Fatemeh Aghaei tested a method for change point detection. This method revealed that the Earth's climate has already passed some tipping points in certain regions.

Complexity measures and brain regions In collaboration with Prof. Estevez from Habana and our PhD student Ania Mesa, we use complexity measures to assess the activation of brain regions during different cognitive tasks and reactions.

Machine learning Following the recent hype in machine learning, we have extended our understanding of the performance of reservoir computing. Reservoir's computing key strength is its simplicity in training: Only the output weights need to be determined by a simple linear regression of the target variable to the internal state. The internal state itself is synchronised with the driving system in terms of generalised synchronisation, which increases the robustness of iterated forecasts. Daniel Estevez, PhD student, reproduced claims from the literature. Together with him and Erick Madrigal, an MSc student, we achieved a major breakthrough in forecasting. Another PhD student, Simon Kneer, used machine learning for symmetry reduction in spatially extended dynamical systems. These are methods to remove, e.g., translational or rotational symmetries from observed data in order to facilitate the analysis of characteristic patterns.

Model error versus growth of initial condition errors As described in detail in Sec.2, small scale motion of the atmosphere is much less stable than large scale motion in terms of much larger Lyapunov exponents. It is therefore not evident that the effort to include ever smaller scales in weather forecasts by improving their spatial resolution is beneficial for long term forecasts. While model error is thereby

reduced, the largest Lyapunov exponent of the model is increased. Together with Hynek Bednar from Prague and a MSc student we are investigating this issue in simplified models.

Future The group leader will retire in roughly 2 years, so that the group will gradually shrink. Already in the past year, no new PhD students were accepted. Instead, research is more and more done by MSc students who will finish their projects before the group leader's retirement.

Collaborations

- Eli Barkai (Bar Ilan, Israel), Aleksei Chechkin (Charkov, Ukraine), Rainer Klages (London, UK), Ralf Metzler (Potsdam, Germany), Trifce Sandev (Skopje, North Macedonia), Erez Aghion (Boston, USA), Kevin Bassler (Houston, USA): Projects related to anomalous diffusion.
- CAFE project: A European ITN on medium range prediction on extreme weather events, coordinated by Alvaro Corral in Barcelona with colleagues from Spain, France, UK, Uruguay, and Germany, including Munich Re as a company. Co-supervising a PhD student at the European Centre for Medium Range Weather Forecast ECMWF in Reading, UK. The project expired in March 2023.
- Benjamin Lindner (HU Berlin, Germany): Multiplicative noise
- Meagan Carney (Brisbane, Australia): Hurricane model, storm tracking, sampling of rare events in dynamical systems.
- Hynek Bednář (Charles University Prague, Czech Republic): Scale dependent error growth and model error in atmospheric models.
- Imre Janosi (Budapest, Hungary) and Jason Gallas (Paraíba, Brasil): Collaboration on oceanic transport.
- Ernesto Estevez Rams (Havana, Cuba): Complexity measures and information metrics for data classification, joint PhD student.

Research Group: Order and Disorder in Driven Systems
(Head: Dr. Marko Popović)

The research group "Order and Disorder in Driven Systems" was established in January 2021. We are interested in understanding how the interplay between patterning, structure, and mechanics of complex materials influences their physical properties. Most of the research in the group revolves around the physics of biological tissues, whose active self-organized dynamics provide a unique playground at which the interplay between mechanics, structural organization and rheological properties takes place. Our research is motivated both by fundamental problems in the physics of non-equilibrium mechanical systems, and through close collaboration with several experimental research groups.

Biological tissues as active amorphous solids In the absence of mechanical or thermal noise, cellular materials are yield stress materials. However, such a description does not account for the activity present in the living systems whereby active cellular processes, such as cell divisions and cell extrusions, introduce fluctuations in mechanical stress. Interestingly, these mechanical fluctuations are fundamentally different from thermal fluctuations as they are driven by biological processes in cells. Therefore, understanding how these processes influence the mechanics and structure of biological tissues requires a dedicated approach that is not a simple extension of equilibrium models. In particular, we study how cell divisions destroy dynamical correlations in developing biological tissues that allow them to be much more effective in fluidising a solid tissue, compared to thermal-like fluctuations. Furthermore, we aim to understand how pressure sensitive removal of cells through cell extrusions imprints a characteristic extreme value statistics of pressure in biological tissues, which can be mapped to the experimentally observable distribution of cell sizes.

Random yielding transition The yielding transition is a dynamical phase transition observed in athermal amorphous solids that plastically flow beyond a critical value of imposed shear stress Σ_c. Recently it was pointed out that the classical yielding transition can be generalized by introducing a finite correlation length in the spatial distribution of the imposed driving stresses, where the homogeneous shear driving corresponds to an infinite correlation length. In this project we use the vertex model of epithelial tissues to study the opposite limit, denoted random yielding transition, in which each cell in the tissue is driven

by an independent randomly oriented cell traction forces. We found that the random yielding transition is described by a set of critical exponents related to the exponents of the classical yielding transition. Furthermore, the study of the random yielding transition allowed us to elucidate experimental observations of complex dynamics of rotating multicellular spheroids observed in experiments by collaborators in the group of Anne Grapin-Botton at MPI-CBG.

Cell size polydispersity controls tissue crystallization Cellular packings in biological tissues are typically disordered during development, which greatly facilitates tissue shape changes. However, in collaboration with the experimental group of Natalie Dye at TU Dresden, we have found that in developing fruit fly wing epithelium cells suddenly reorganize into an ordered state with a large number of almost perfectly ordered hexagonal crystallites. In this project we use experimental data analysis and simulations of a model of epithelial tissues to propose that this transition is controlled by the distribution of cell sizes. Crystallization can only occur if cell sizes are sufficiently uniform so that a hexagonal cell packing becomes the ground state of the system.

Regeneration of Hydra Hydra is a freshwater animal that exhibits extraordinary regeneration potential, and can regenerate from a small fragment excised from a parent animal. During the regeneration process, the tissue fragment initially folds into a spheroid, undergoes repeated contractions due to muscle activation and finally forms a head on one side and a foot on the opposite side, breaking the apparent symmetry of the original fragment. Interestingly, this regeneration process is very robust to perturbations, but sometimes a Hydra with multiple heads can emerge if regeneration is sufficiently frustrated. In this project we work with the experimental group of Kinneret Keren to understand the principles underlying Hydra regeneration that combines tissue mechanics, large-scale organization of nematic muscle fibers and tissue excitability through calcium signalling.

Tissue folding as a morphogenetic mechanism How an animal tissue grows and physically shapes itself into its final form remains an exciting and important open question in both developmental biology and biophysics. We propose that epithelial tissue folds can serve as active, self-organized boundaries that are critical for the oriented growth and morphogenesis of surrounding tissue. This phenomenon is exemplified by the fruit fly *D. melanogaster* imaginal disc epithelium. Folds in this epithelium are transient, and unfold as the tissue remodels into a shape resembling the final wing form. This behavior contrasts with other previously studied examples of tissue folding, e.g. the vertebrate gut or brain, whose folds are stable and have a biological function in the mature tissue. In this project we work with the experimental group of Natalie Dye to address whether and how transient tissue folding could function as a morphogenetic mechanism.

Theoretical collaborations:

- Matthieu Wyart (EPFL, Lausanne, Switzerland) on activated flow of amorphous solids
- Frank Jülicher (mpi**pks**, Dresden, Germany) on mechanics and patterning of developing fruit fly wing and active rotations of cellular spheroids

Experimental collaborations:

- Natalie Dye (Physics of life, TU Dresden, Germany) on mechanics and patterning of developing fruit fly wing and tissue folding
- Kinneret Keren (Technion, Haifa, Israel) on mechano-chemical dynamics of Hydra regeneration
- Anne Grapin-Botton (MPI-CBG, Dresden, Germany) on active rotations of cellular spheroids

Research Group: The Physics of Living Matter
(Head: Dr. Ricard Alert)

Living matter is active: It is driven away from thermodynamic equilibrium by its own constituents — be they molecular motors in the cell, bacteria in a colony, or organisms in a herd. How does this internal driving impact the exquisite organization of living matter? How do collective phenomena in biological systems emerge from the active nature of living matter? Our group seeks to understand collective

behaviors in cells and tissues through the lens of active matter physics. To this end, we collaborate closely with experimentalists to identify physical principles and mechanisms that underlie specific biological processes, such as cell migration, embryo implantation, and the multicellular organization of bacterial colonies. Beyond biological systems, we also develop more general aspects of the physics of active matter by combining ideas from statistical physics, soft matter, and fluid dynamics. Along these lines, we study turbulent-like flows in active fluids, phase transitions in suspensions of self-propelled particles, and non-equilibrium fluctuations in active gels. Our work on these topics is outlined below.

Guidance of cell migration. Cells migrate to find their place in a developing embryo, to heal wounds, and to invade other tissues during cancer metastasis. But how do they find their way? In collaboration with the lab of Roberto Mayor at University College London, we study how cells can use not only chemical but also mechanical signals to orient their migration. The experiments by our collaborators showed that cells in microchannels migrate towards stiffer environments — a process known as durotaxis — even if they do not adhere to the channel walls. To understand this puzzling observation, we proposed that cells actually follow gradients of substrate friction — a process that we called frictiotaxis. We demonstrated this process by means of a model of the cellular cytoskeleton as an active gel. Our collaborators then confirmed that cells perform frictiotaxis in experiments. The discovery of this new mechanism of cell guidance motivates us, in collaboration with the group of Sebastian Alland at TU Bergakademie Freiberg, to explore further ways of guiding the migration of non-adherent cells, for example via channel topography, pressure, and the interaction with nearby cells.

Collective cell migration. In development, regeneration, and cancer, cells often migrate in cohesive groups. How do individual cells coordinate their motion with others? And how do cell aggregates change their shape as they migrate? In collaboration with the lab of Xavier Trepat at the Institute for Bioengineering of Catalonia, we study how cell aggregates break symmetry to migrate collectively, how they spread on substrates, and how they move towards stiffer environments — a process known as collective durotaxis. To this end, we develop models of cell aggregates as active liquid droplets that follow generalized laws of wetting. We also apply these physical principles to instances of collective cell migration in vivo, such as mouse embryo implantation in collaboration with Kate Cavanaugh at the University of California San Francisco, and the development of the frog head in collaboration with the lab of Elias Barriga at the Cluster of Excellence Physics of Life at TU Dresden. Key questions that we are addressing are: Which mechanical properties are responsible for the impaired spreading of embryos from older mothers? How do gradients in the mechanical properties of cell clusters guide their migration? How do events of cell division affect the migration of cell clusters?

Multicellular organization of bacterial colonies. The motile soil bacterium *Myxococcus xanthus* lives in colonies of millions of individuals that organize differently depending on environmental conditions. When there are nutrients around, *M. xanthus* colonies form a monolayer where the rod-shaped cells align with one another forming an active nematic liquid. When they starve, these bacteria form additional cell layers at the location of nematic topological defects, which enable them to build three-dimensional structures called fruiting bodies, where the bacteria turn into spores to survive in the absence of nutrients. How do bacteria control their collective organization? We break this general question down into smaller, more specific ones. For example, how do cells aggregate into a dense nematic monolayer in the first place? In collaboration with the lab of Joshua Shaevitz at Princeton University, we discovered that cells are wet by a meniscus of water extracted from their porous substrates, which makes them attract via capillary forces. Motivated by this finding, we are developing a theory for self-propelled particles with capillary interactions — a class of active systems that we call hydrated active matter. From a nematic cell layer, how do new cell layers form at topological defects? We are developing a theory of layer formation as a nucleation process in which the energy barrier fluctuates due to stochastic cell motility, which creates pressure fluctuations in the colony. Finally, experiments also revealed ripples at the upper surface of thick colonies of *M. xanthus*. We are developing a theory for these ripples as height waves at the surface of an active nematic film. Again, the presence of water wetting the colony is key to understanding the physical origin of this striking collective phenomenon.

Active turbulence. Ordinary turbulence occurs at high Reynolds numbers due to inertial effects. Strikingly, active fluids display turbulent-like flows at very low Reynolds numbers — a phenomenon known as active turbulence. Previous work showed that active and inertial turbulence exhibit key similarities, such as the existence of scaling regimes in the kinetic energy spectrum, but also fundamental differences, such as the lack of an energy cascade in active turbulence. Do other key features of inertial turbulence carry

over to its active counterpart? We address this broad question in a few different directions, focusing on active nematic fluids. First, how does active turbulence emerge from laminar flows? We discovered that, in the absence of confinement, the transition to active nematic turbulence is discontinuous, and it exhibits a jump in flow intensity, bistability, and hysteresis. We also study active turbulence on a substrate, which is relevant for many experimental systems such as bacterial and epithelial cell layers. Here, we ask how the spectrum of turbulent flow is affected by substrate friction and active cell-substrate forces. Finally, we also address the problem of mixing by active turbulence, which has implications for the design of active microfluidic devices. Here, we study the concentration spectrum of a passive solute mixed by active turbulent flows.

Phase transitions in active matter. Active matter can organize itself in ways not possible at thermodynamic equilibrium. In addition to undergoing turbulent-like flows in the absence of inertia as discussed above, self-propelled particles can phase separate even if they repel each other, and they can achieve long-range orientational order in two dimensions. These phenomena, respectively known as motility-induced phase separation and flocking, are landmark phase transitions induced by activity. How does activity enable such phase transitions? And which mechanisms underlie these transitions in specific systems? In collaboration with the lab of Jie Zhang at the University of Science and Technology China, we address this question in a model system made of self-propelled colloids driven by electric fields. Whereas most work on active particles has focused on either excluded-volume or alignment interactions, our colloids interact electrostatically in a way that makes them turn either towards or away from one another. We discovered that such active colloids can flock together even if they turn away from one another. We then used theories from non-equilibrium statistical mechanics to understand the mechanism behind this phenomenon. We now explore whether the same mechanism might underlie flocking in cells, which turn away from one another upon collision in a behavior known as contact inhibition of locomotion. In collaboration with the group of Marín Bukov at mpi**pks**, we are also studying the collective behavior of active colloidal dimers, which could potentially undergo flocking and phase separation simultaneously.

Active fluctuations. Living matter is internally driven by irreversible processes such as the action of molecular motors. Thanks to theoretical work in the past two decades, we now have hydrodynamic theories of active materials, which are being fruitfully applied to biological systems. So far, these theories have focused mostly on the *average* effects of activity. However, active processes also generate prominent non-equilibrium fluctuations, which are fundamentally different from equilibrium thermal fluctuations and impact biological processes such as intracellular transport. What are the statistical properties of active fluctuations? In collaboration with Frank Jülicher at mpi**pks**, we are developing a theoretical framework to derive the noise terms in hydrodynamic equations of active gels. By explicitly coarse-graining a specific model of cytoskeletal networks, we connect the spectrum of active noise to the breaking of detailed balance that captures irreversibility in the binding kinetics of cytoskeletal proteins. Through these calculations, we aim to generalize the fluctuation-dissipation relation to include the additional effects of activity.

Research Group: Transport and Flows in Complex Environments

(since May 2022, Head: Dr. Christina Kurzthaler)

The group "*Transport and flows in complex environments*" was established in May 2022 as a Max Planck Research Group. Our research deals with the physics of soft materials driven far from equilibrium with a particular focus on transport phenomena in active matter systems. Recent advances in microfluidics and microscopy allow building new platforms for studying biological systems across several scales. Bridging experimental observations with our theoretical predictions has proven vital for identifying physical laws governing their complex dynamics. In our work, we study how the environment, imposing geometric constraints, hydrodynamic and chemical fields, shapes transport processes and self-organization of microorganisms and subcellular constituents. Our research further aims at leveraging biophysical concepts for designing new inanimate materials. To investigate these research themes, we use analytical and computational tools from statistical physics and fluid mechanics and closely interact with our experimental colleagues. Here we outline our main research topics.

Spatiotemporal characterization of active agents To optimize their survival, microorganisms have evolved a large variety of ingenious strategies allowing them to efficiently forage food and proliferate in seemingly unhabitable niches, omnipresent in their diverse habitats, such as soils, the ocean, or the

human body. Many microorganisms are able to self-propel through their complex surroundings, providing them an indispensable advantage over transport via ordinary diffusion. We are interested in unraveling the intricate physics of this active transport behavior, which displays a range of unusual, out-of-equilibrium phenomena. The paradigmatic example of a biological active agent is the bacterium *E. coli*, whose biochemistry and genetics have been extensively studied while the spatiotemporal characterization of its dynamics and a direct link to the functioning of the bacterial motor have remained a challenge. We have shown that using a combination of theoretical predictions based on renewal theories and experimental measurements of the intermediate scattering functions, quantifying the dynamics over several length and time scales, represents a new, powerful method for establishing a profound understanding of the underlying physics. Extending this framework, by developing new theoretical models, we are paving the way for quantitatively studying the swimming gait of various microorganisms and their response to external (for example, chemical) cues. Our analytical work further centers on first-passage-time properties of active agents to reach desired targets, a question that is paramount in biological systems, ranging from sperm cells finding the egg to specific target binding to DNA.

Hydrodynamics of swimming in confinement Many microorganisms live in aqueous environments where interactions with nearby confining boundaries lead to interesting features that greatly differ from their passive counterparts, due to the intricate flow fields produced by their swimming mechanisms. Interactions between microswimmers and surfaces composed of different materials can be of, amongst others, chemical, electric, steric, or hydrodynamic origin. Unraveling the contributions is an important aspect of our understanding of the complex aggregation of bacterial communities near surfaces. While much is known about the interactions of microswimmers with planar walls, our understanding of active transport near structured and deformable boundaries, such as biological membranes, is sparse. The latter involves complex elastohydrodynamic couplings between the active agents and the boundary, which can profoundly change the near-surface dynamics and, consequently, may impact the formation of bacterial colonies. We use analytical theories, based on perturbation theories and the Lorentz reciprocal theorem for Stokes flows, together with new numerical tools relying on the "multiblob" approach to elucidate these questions. We therefore investigate the dynamics of different microswimmers and aim to include the aspect of noise for studying the impact of hydrodynamics and surface properties on first-passage-time statistics.

In this context, our work further addresses the motility of sperm cells under various environmental conditions, including non-Newtonian fluid behaviors and chemical fields, that mimic the complex environment of the female reproductive tract. We combine experimental observations, statistical profiling of cell motion, and hydrodynamic theories to unravel the main features of transport of sperm cells under these conditions, thus bridging the gap towards real applications.

Flows and active transport in porous media Fluid transport through complex media plays a fundamental role in diverse areas, ranging from modern technological applications to geophysics to biology. In heterogeneous environments, fluid flow encounters highly disordered porous structures with many dead-end pockets and corners, yielding numerous regions of stagnant flow alongside a few pores of rapid fluid streams, rendering it an exciting topic at the interface of fluid mechanics and statistical physics. Several fundamental questions for various fields remain still open, which we tackle from distinct perspectives. First, our group addresses the physics of Stokes flow through porous media at the percolation transition, revealing power-law behaviors of the flow rate near the critical point (obtained via extensive numerical simulations). Second, we study the impact of these heterogeneous flows and confinement on the active motion of agents, to fully elucidate the spreading of microorganisms in dense environments. Our first results suggest that the interplay of swimming motion and fluid shear leads to rheotactic behavior and enhanced trapping of the agents in dead-end-pores with robust power-law trapping-time distributions. We aim at identifying universal principles across various microorganisms and revealing optimal strategies for their survival in such complex surroundings.

Phoretic active matter Prominent examples of synthetic active agents are phoretic colloids. Much research has focused on spherical colloids and their collective effects, including the emergence of non-reciprocal interactions through hydrochemical coupling of the agents. Relaxing the constraint of spherical shapes, our goal is to shed light onto the motion of slender phoretic objects and their interactions with boundaries and others. These insights could provide fundamental ingredients towards tailoring and designing new adaptive active materials.

Theoretical collaborations:

- Thomas Franosch (U Innsbruck, Austria): Statistical Physics of Active Transport
- Hartmut Löwen (U Düsseldorf, Germany): Entangled Active Polymers
- Suvendu Mandal (U Darmstadt, Germany): Transport in Porous Media, Entangled Active Polymers
- Julien Tailleur (MIT, United States of America; U Paris, France): Bacterial Motion
- Axel Voigt (TU Dresden, Germany): Porous Media Flows

Experimental collaborations:

- Sujit S. Datta (Caltech, United States of America): Bacterial Transport in Porous Media
- Daniela J. Kraft (U Leiden, Netherlands): Phoretic Anisotropic Colloids
- Vincent A. Martinez (U Edinburgh, United Kingdom): Bacterial Motion
- Juliane Simmchen (U of Strathclyde, United Kingdom): Phoretic Colloids in Porous Media
- Howard A. Stone (Princeton U, United States of America): Microfluidics, Sperm Motility

Awards of people in the group:

- Pallabi Das: Alexander von Humboldt Research Fellowship (co-supervised with Suvendu Mandal, TU Darmstadt, Germany)
- Akhil Varma: Alexander von Humboldt Research Fellowship (co-supervised with Frank Jülicher, mpi**pks**)

1.9 Groups

Research Group: Self-Organization of Biological Structures
(until November 2022, Head: Dr. Jan Brugués)

The group Self-organization of biological structures started in September 2013 and aims to uncover the principles of how cellular compartments emerge from the collective behavior of individual molecules. Current research in my group is centered around two general questions, both aiming at understanding the emergence of cellular compartmentalization. First, we are studying how the size and shape of spindles arise from the interplay of mechanics, microtubule nucleation, and motor activities, and how these properties are regulated during early development and determine cytoplasmic compartmentalization. Second, we want to understand the principles that govern active chromatin organization in the nucleus, a question that has been largely ignored from the physical point of view. My group has shown key aspects of microtubule nucleation, spindle shape and mechanics, and scaling in embryos and artificial cell-like compartments. We have provided the first direct proof of DNA loop extrusion in a cellular context by reconstituting and visualizing this process on single DNA molecules in cell extracts using single molecule microscopy. We also have shown that capillary forces driven by transcription factors lead to the emergence of DNA condensates, providing a new physical principle that could explain how distant DNA sequences meet to initiate and regulate transcription in the nucleus. Both research directions synergize and benefit from our strong expertise in theory, quantitative microscopy, biophysical approaches, and reconstitution. Below I provide a description of the most relevant research areas we currently investigate.

Mechanisms of spindle scaling and orientation. Reductions in cell size during early animal development require that intracellular structures adjust their size accordingly. The mitotic spindle is a microtubule-based structure that robustly segregates chromosomes over a large range of cellular volumes. However, we still lack a mechanistic understanding of the microtubule-based processes regulating spindle relative to cell size. We developed a high-resolution microscopy-based assay to systematically quantify, for the first time, microtubule dynamics, nucleation and 3D organization in spindles over a large range of sizes in early zebrafish embryos. We discovered a hierarchical regulation of spindle scaling with cell size. In large cells, microtubule nucleation exclusively scales spindle size relative to cell size by changing the number of microtubules. In small cells, microtubule-dynamics additionally fine-tune spindle size by modulating microtubule length, though not sufficiently to account for spindle scaling alone. Our data, in combination with theory, support a model in which component limitation of microtubule nucleators and membrane

partitioning of a nucleation inhibitor quantitatively explains both the exact scaling of spindles with cell size, and also the hierarchical regulation of microtubule nucleation and dynamics. In the future, we want to use the methods we developed to reconstitute the early embryo reduction divisions using encapsulated cycling egg extracts in physiological membranes. These extracts self-organize into 'cell-like' compartments that partition the cytoplasm and autonomously go through the cell cycle forming large-scale mitotic waves that lead to surprisingly uniform partitioning. These experiments in combination with theory will allow us to dissect the physical principles that mediate spindle scaling, how the orientation of spindles and their centering depends on geometrical cues, and what self-organization principles determine the patterns of actin and microtubules in the cell boundary.

Theory and simulations of spindle morphology. The combination of theory and experiments allowed us to show that microtubule nucleation is autocatalytic and spatially regulated. These findings on microtubule nucleation show that previous models of spindle assembly are incomplete and suggest a mechanism of spindle formation that resembles classic Fisher-waves and Turing mechanisms. However, our mechanism has the fundamental difference that microtubule autocatalytic waves do not require diffusion or advection to propagate. Instead they are a consequence of the finite extension and dynamics of the reactant (the microtubule). For example, this phenomenon leads to self-organized patterns of microtubule growth in autonomously cycling extracts, with wavelengths similar to an embryo, suggesting a limit of how spatial information can be transmitted and synchronized in embryos. Similarly, we have shown that material properties in spindles are key to understanding microtubule flows in Xenopus egg extract spindles. In particular, we have shown that spindles undergo a sol-gel transition that is essential to drive polarity-independent flows and propagate stresses throughout the structure. Our work starts to provide a unified view of how self-organized flows are generated in the spindle. In the future, we will incorporate motor activities and autocatalytic microtubule growth into a continuum theory and a microscopic simulation that recapitulates not only the assembly of the entire spindle and scaling but also explores the phase space of the interplay between motor activities and autocatalytic growth in determining spatial compartmentalization driven by mitotic waves.

The role of transcription factor-mediated capillary forces in organizing chromatin. Proximity of enhancer regions and gene promoters drive transcription in cells and embryos. However, how transcription factors, co-factors, and general transcriptional machinery work in concert to physically cluster DNA remains unclear. We have developed a new assay that combines quantitative microscopy and in vitro reconstitution to visualize the interactions between single DNA molecules and the pioneering transcription factor FoxA1. Using this assay we have shown that FoxA1 binds DNA and can mediate the nucleation of DNA condensates via a first-order phase transition. Surprisingly, after formation, DNA condensates exert capillary forces on the remaining non-condensed strand. These findings could represent a possible mechanism to facilitate enhancer–promoter contacts, and play a more general role in DNA compaction and chromatin rigidity. However, the physics of protein-DNA condensation in the chromatin fiber are completely unexplored. In the future, we aim to investigate protein-DNA co-condensation in the context of single molecule chromatin: how chromatin influences capillary forces, size and nucleation of condensates; how condensation affects the specificity of transcription factors; and how different types of condensates compete for available chromatin.

Physical mechanisms of DNA loop extrusion reconstituted in single DNA molecules. Loop extrusion by structural maintenance of chromosomes complexes (SMCs) has been proposed as a mechanism to organize chromatin during the cell cycle. However, the requirements for chromatin organization in these cell phases are very different, and it was unknown whether loop extrusion dynamics and the complexes that extrude them also differ. We used Xenopus egg extracts to reconstitute and image for the first time loop extrusion of single DNA molecules in a cellular context during the cell cycle. Our work showed that loop extrusion is a general mechanism for the organization of DNA, with dynamic and structural properties that are molecularly regulated during the cell cycle. However, in light of our discovery of transcription factor-mediated DNA condensation—that generate similar forces—these two mechanisms may self-organize in the nucleus. For example, protein-mediated DNA condensation may act as a roadblock and interfere with loop extrusion. Alternatively, loops formed may be further stabilized by capillary forces within the loop. We will use our assays to investigate the interplay between these two processes, and extend our theory of protein-DNA co-condensation to include activity driven by loop extrusion. The synergy between transcription factor-mediated DNA co-condensation and loop formation may be a general mechanism to organize transcription in the nucleus. Because cell extracts are transcriptionally active upon titration of nucleosomes, these experiments will allow to increase the complexity of our experimental system to

reconstitute chromatin domains, and to correlate loop formation with gene expression.

Characterizing emergent properties of chromatin reconstituted in synthetic nuclei. We have developed an assay to reconstitute functional nuclei in encapsulated extracts (synthetic nuclei). We aim to use this assay in combination with quantitative imaging and mechanical measurements, to understand how molecular activities give rise to the emergent physical properties of chromatin. Our assay allows to precisely control the amount of genetic material per synthetic nucleus, titrations of components, and size of synthetic nuclei. Tuning the length of DNA will allow to investigate whether the viscoelastic behaviors of synthetic nuclei scale with polymer length as expected from equilibrium polymer physics and how those behaviors deviate in the presence of active chromatin processes. To study emergent physical properties of chromatin from molecular activities, we aim to combine passive two-point microrheology and active rheology measurements in chromatin. However, combining this type of measurements in cells is challenging, and has not been performed in chromatin. We will exploit mechanical accessibility of extracts to disentangle active and passive contributions to the physical properties of chromatin by combining two-point microrheology with active rheology. As an ultimate goal to this research line, we will investigate the impact of chromatin material properties and DNA-condensation on transcription by reconstituting it in synthetic nuclei.

Collaborations

- Nadine Vastenhouw (University of Lausanne, Switzerland)
- Christoph Zechner (CSBD Dresden, Germany)
- Tony Hyman (MPI-CBG Dresden, Germany)
- Stephan Grill (MPI-CBG Dresden, Germany)
- Frank Jülicher (mpi**pks** Dresden, Germany)

Max Planck Research Group: CSBD - Self-Organization of Multi-cellular Systems
(Head: Dr. Pierre Haas)

The Max Planck research group "Self-Organisation of Multicellular Systems" was established at mpi**pks** in January 2021, and is jointly affiliated with MPI-CBG and based at the Center for Systems Biology Dresden. The theoretical research of the group focuses on the biomechanics of cell sheets and their regulation in development and spans close collaborations with experimental groups in Dresden and farther afield as well as more abstract physical questions inspired by these biological problems. This research programme divides into two strands:

(Continuum) Mechanics of Biological Tissues. During development, the functional shapes of tissues, organs, and organisms emerge from processes of tissue folding driven by the cell scale. In particular, understanding this morphogenesis requires understanding the mechanical forces that drive this tissue folding. In turn, and more physically, this presupposes understanding the constitutive laws that describe the mechanical behaviour of tissues. However, biological tissues need not obey the constitutive equations of classical continuum mechanics, not only because living systems are active and out of thermodynamic equilibrium, but also because of (i) large geometric deformations or internal rearrangements specific to these biological materials, and (ii) constitutive peculiarities resulting from the underlying cell-level mechanics. How mechanical forces shape tissues and how tissue-scale rheology emerges from cell-scale mechanics are therefore fundamental biological and physical questions, which we explore in different experimental systems and minimal physical models.

Biomechanics of development. In this context, we have studied, for example, how mechanical forces from the coupling of neighbouring tissues shape the developing zebrafish forebrain [collaboration with Michael Smutny (University of Warwick)]. A particular focus of our recent work has been on mechanical bifurcations or instabilities: For instance, we have described a mechanical instability of the shape of the extending *Drosophila* germband [collaboration with Pavel Tomančák (MPI-CBG)]. We have also shown how a mechanical bifurcation selects the shape of the hindgut primordium of *Drosophila* [collaboration with Stas Shvartsman (Princeton University / Flatiron Institute)].

Inference of mechanical properties. "Cutting" and "poking" assays give access to the mechanical properties of and forces in biological tissues, but, importantly, need a quantitative mechanical model that relates the recoil on laser ablation ("cutting") or the displacement on AFM indentation ("poking") to these

mechanical properties. In this context, we have shown how to infer out-of-plane forces in curved tissues from laser ablation experiments in the green alga *Volvox* [in a long-standing collaboration with Steph Höhn (University of Cambridge)] and how cell contractility and nonlinear elastic rheology give rise to new scaling exponents in the force-displacement relation of cyst indentation experiments. Our future work in this area will seek out the signatures of more complex material behaviour, such as non-local elasticity, in these assays.

Continuum mechanics of epithelial tissues. These and other experimental systems also raise more fundamental mechanical questions, which we study in minimal models inspired by these systems. Examples in our recent work include a continuum description of plastic tissue deformations via cell rearrangements inspired by the serosa closure process of the beetle *Tribolium* or the "(un)buckling" of tissue folds that provides a mechanism for tissue folds such as the cephalic furrow in *Drosophila* to absorb compressive stresses from neighbouring tissues. Spontaneous wrinkling instabilities of tissues, associated with cell-scale asymmetry from apicobasal polarity for instance, constitute one direction for our future work in this area.

Hydraulics and signalling dynamics in morphogenesis. We also contribute more widely to developing a minimal physical framework of the interplay of hydraulics and mechanics in morphogenesis, through ongoing collaborations on the development of the network of bile canaliculi in the liver [with Marino Zerial (MPI-CBG / Human Technopole)] and on the morphogenesis of the *C. elegans* gonad [with Stephan Grill (MPI-CBG)]. We are now also beginning to add mechanochemical feedbacks and morphogen signalling into this mix, in particular in a collaboration with Jacqueline Tabler (MPI-CBG) on cell differentiation during mouse brain development.

Robustness and Variability of Development. How is robust development compatible with the huge variability of biological systems? This is a fundamental biological problem, and the mechanisms underlying the exquisite precision of morphogen signalling have indeed been analysed in detail, but the interplay of cell-scale disorder and mechanics remains poorly understood. For this reason, it is largely unknown how robust morphogenesis emerges at the tissue scale. In fact, it is even unknown in most cases how close morphogenetic processes get to their mechanical limits. We have recently quantified this for the inversion process of *Pleodorina*, which enabled us to show how a mechanical bifurcation constrains the evolution of cell sheet folding in these green algae.

Statistical continuum mechanics. To begin to ask how cell-scale disorder affects tissue-scale mechanics more generally, we have recently extended the classical buckling problem of a rod that is growing against clamped ends by adding quenched disorder to this growth. Finite-element simulations revealed rich (and sometimes counterintuitive) effects on the buckling threshold. In particular, while such microscopic disorder would average out at a coarse-grained scale in linear problems, this cannot be expected to be the case in nonlinear problems such as buckling. Analytical understanding of this behaviour requires, however, a theory of "statistical continuum mechanics" that shows how this microscopic disorder of growth strains or analogous disorder of mechanical parameters adds statistical moments of the distributions of these parameters at the continuum scale. We are now starting to derive such a theory and to study these continuum mechanics with disorder more generally. This opens up a large research programme, in which feedbacks of mechanical stresses on disorder constitute but one additional direction for future work.

Beyond this core interest, the group has a side interest in problems of theoretical ecology and more abstract problems related to the physics of complex systems.

Dynamics of Ecological Communities. Fifty years ago, May argued that random ecological communities are overwhelmingly likely to be unstable. Ever since, theoretical ecology has been seeking to identify those structures that allow actual ecological communities to overcome this statistical constraint.

Theoretical Ecology of Phenotypic Variation. In this context, our work has focused specifically on the effect of subpopulations, associated with phenotypic variation, on stability of coexistence in ecological communities. In particular, we have shown that phenotypic switching in response to competitors has a rich effect on stability even in minimal two-species models in which purely stochastic phenotypic switching has no effect on stability. More recently, we have analysed the effect of phenotypic switching on the travelling waves by which one species invades another in this two-species model.

"Impossible" and "irreducible" ecologies. We have recently analysed the effect of the network of ecological interactions on stability of coexistence by exhaustive sampling of all networks of competitive, mutualistic, and predator-prey interactions of $N \leqslant 5$ species with Lotka–Volterra dynamics. This full

effect of this network structure remained inaccessible in random-matrix-theory approaches *à la* May, but our work shows that this effect can be huge, in particular by discovering exponentially rare "impossible" ecologies (in which stable coexistence is non-trivially impossible) and similarly rare "irreducible" ecologies that determine the possibility of stable coexistence in larger communities completely. Our future work will seek similar descriptions of more complex dynamics beyond steady state, starting from an analysis of limit cycle dynamics in these systems.

Experimental collaborations

- Stephan Grill (MPI-CBG), on the mechanics and hydraulics of the morphogenesis of the *C. elegans* gonad;
- Steph Höhn (University of Cambridge), on the inversion of the alga *Volvox*;
- Alf Honigmann (TU Dresden), on the biomechanics of cysts;
- Stas Shvartsman (Princeton University / Flatiron Institute), on the morphogenesis of the *Drosophila* hindgut;
- Michael Smutny (University of Warwick), on the fluid mechanics shaping the zebrafish forebrain;
- Jacqui Tabler (MPI-CBG), on cell differentiation during brain development;
- Pavel Tomančák (MPI-CBG), on the mechanics of germband extension in *Drosophila*;
- Marino Zerial (MPI-CBG / Human Technopole), on the mechanics of bile canaliculi formation during liver development.

Research Group: Statistical Physics of Living Systems
(until September 2022, Head: Dr. Steffen Rulands)

The Statistical Physics of Living Systems group uses methods from theoretical physics to study novel forms of non-equilibrium matter. These forms of non-equilibrium matter arise from recent technological developments in various fields of science.

Intelligent matter Firstly, we study self-organization and emergence in intelligent matter. The recent rapid advances in artificial intelligence have led to scientific breakthroughs in fields as diverse as quantum simulation and protein design. The cornerstone of these advances is deep neural networks, mathematical models comprising nonlinear nodes that are linearly connected by weights and exist in various architectures. Composite systems are emerging in the field of robotics, in which collections of "intelligent" agents interact to fulfil specific tasks. But are such artificial intelligence systems just complicated ways of doing curve fitting, or can they exhibit new behaviour that goes beyond the bounds of the data that is used to train them? Whether artificial intelligence systems can exhibit emergent behaviour, and if so, how, is not only of fundamental interest to the machine learning theory but also crucial for estimating potential security risks of increasingly capable artificial intelligence systems. Empirical studies have found signatures of emergent capabilities in very large neural networks, such as the abrupt development of new capabilities over time or as one increases their size. As a further example, a study on a large language model trained entirely on text suggested internal spatial representations of objects. Starting from the known microscopic rules governing parameter and activity updates we develop first-principle theories of emergent phenomena in deep neural networks. Inspired by robotics, we also investigate the behaviour of stochastic gases of interacting deep neural networks. These systems lack microscopic symmetries and exhibit emergent symmetries as well as phase transitions and critical behavior.

Genomic matter Recent technological breakthroughs in biology have given unprecedented access to molecular states of cells. For the first time, it is now possible to obtain information on the expression of thousands of genes, on epigenetic modifications of the DNA on single loci, and on the spatial organisation of chromatin of thousands of single cells from living organisms. Single-cell multi-omics technologies allow profiling of several layers of regulation in the same cell. These technological developments have led to detailed descriptions of the molecular processes underlying cellular behaviour. Biological function, such as cell differentiation, proliferation or death, however, is determined by emergent (collective) states on the cellular and tissue scale which arise from interactions between processes occurring at many different loci on the molecular scale. But how can detailed quantitative information on the microscopic scale inform on emergent processes that determine biological function at the cellular and tissue scale? We use and develop methods from non-equilibrium statistical physics to infer the collective, mesoscopic phenomena

that underlie cellular function from single-cell sequencing experiments. We apply these approaches to understand collective epigenetic phenomena during ageing, rejuvenation and regeneration.

Multi-scale matter Understanding how fluctuations propagate across spatial scales is the foundation of theories of inanimate matter. For example, in turbulence, velocity fluctuations induced on the macroscopic scale propagate to the microscopic scale and dissipate there. In critical phenomena, fluctuations propagate self-similarly from the microscopic to the macroscopic scale, leading to divergences in thermodynamic response functions. Understanding these phenomena requires theoretical methodologies in the form of renormalization group theory or coupled modes theory, which allow for calculating the emergent effect of all intermediary scales on physical properties of interest. In contrast to inanimate matter, biological systems are organized into a discrete hierarchy of non-equilibrium processes on vastly different spatial scales. Molecular processes are often embedded into subcellular structures termed organelles and cells interact to form complex organs that constitute organisms. We develop statistical physics and thermodynamic theories for the propagation of fluctuations across biological scales. We also investigate how biological systems use this architecture to perform biological functions such as signal processing. For example, we recently showed that multi-scale dynamics give rise to quasi-particles in the space of chemical concentrations which is used by cells to construct a low-pass filter controlling cell death.

Collaborations

- Wolf Reik, Altos labs and Babraham Institute, Cambridge (UK) on theories of DNA methylation and gene expression dynamics during embryonic development and ageing
- Philipp Mergenthaler, Charité Berlin (Germany) on the multi-scale regulation of neuronal cell death
- Meri Huch, MPI-CBG, Dresden (Germany) on liver regeneration
- Maximina Yun, CRTD, Dresden (Germany) on ageing and regeneration in axolotl
- Michaela Fre, Institut Curie, Paris (France) on breast cancer initiation
- Maria Pilar Alcolea, Cambridge Stem Cell Institute, Cambridge (UK) on tumor evolution and ageing
- Solenn Patalano, BSRC Institute "Alexander Fleming", Athens (Greece) on self-organisation of specialisation and plasticity in social insects
- Daniel Stange, Universitätsklinikum Dresden, Dresden (Germany) on the development of machine-learning methods for personalised cancer therapies

Max Planck Research Group: Fractionalization and Topology in Quantum Matter

(until September 2022, Head: Dr. Inti Sodemann)

The research group Fractionalization and Topology in Quantum Matter was established at the mpi**pks** since September 2017, and its last member (doctoral student Nikolaos Stefanidis) successfully defended his PhD in April of 2024. During this period we succesfully trained and graduated four PhD students (Oles Matsyshyn, Sebastian Mantilla, Peng Rao, and Nikolaos Stefanidis) and developed multiple scientific projects with postdoctoral researchers (including Falko Pientka, Li-kun Shi, Zhenjiu Wang, Chuan Chen, Po-Yao Chang, Jun-Yong Khoo, Suraj Hegde), visiting students (including Urmimala Dey, Snehasish Nandy, Jonah Herzog-Arbeitman), as well as with other group leaders and scientists at the Institute (including Francesco Piazza, David Luitz, Roderich Moessner).

Our work deals with the interplay of strong interactions and topology in quantum matter. Our studies fall within four broad categories: (a) non-equilibrium open and driven quantum many particle systems, (b) quantum transport, dynamical and optical phenomena involving Berry's phase, (c) fractionalized and topological phases of matter, particularly spin liquids and quantum Hall systems, and (d) non-perturbative approaches to strongly interacting phases of gapless fermions. We summarise below some of the recent research projects and findings over the last few years which are new relative to the previous scientific report:

Non-equilibrium quantum liquids of periodically driven fermions. Our recent investigations have revealed that the non-equilibrium steady states of periodically driven fermions can retain sharp fermi surfaces and remain much more quantum than previously anticipated. We found that, interestingly, the non-equilibrium steady states of fermions can be very different in a grand-canonical setting where the system exchanges particles and energy with the bath (i.e. fermions coupled to a fermionic bath) and a canonical setting where the system only exchanges energy with the bath (i.e. fermions coupled to a bosonic bath). In the grand-canonical setting there is a non-equilibrium Fermi-liquid-like steady state

with an occupation that displays multiple jumps resembling a staircase shape, and therefore features multiple non-equilibrium Fermi surfaces. In contrast, in the canonical setting there is a non-equilibrium non-Fermi-liquid steady state where the occupation does not have jumps but rather multiple sharp kinks, which, remarkably, remain sharp even when the bath is at finite temperature.

Anyon polaron problems in spin liquids. We have systematically investigated the evolution of the anyon quasiparticles of the Kitaev model perturbed by a Zeeman field away from its exactly solvable limit in order to gain insights on the competition of its chiral spin liquid and nearby phases, such as the mysterious intermediate phase observed in the antiferromagnetic model. We studied all of its anyon quasiparticles types: the non-abelian visons, the fermions and the local bosons. Both for the ferro- and antiferro-magnetic models we found that several quasiparticles become gapless at nearly identical critical values of the Zeeman coupling. This provides evidence for the realization of non-trivial phase transitions. In the anti-ferromagnetic model this also implies that previous theories of the intermediate phase, viewed as a spin liquid with a different Chern number for the fermions, are inadequate, as they presume that the vison gap does not close. Furthermore, in the antiferromagnetic Kitaev model we also found that a local bosonic quasiparticle becomes gapless at nearly the same critical Zeeman field at which the visons and fermions become gapless. This boson carries the quantum numbers of an in-plane anti-ferromagnetic order parameter, raising the possibility that intermediate mysterious phase has spontaneously broken symmetry with this order.

Theory of the fractional quantum spin Hall state in moire materials. We have proposed a theory for the fractional quantum spin Hall effect discovered experimentally in MoTe2. We have shown that a strongly correlated state of electrons and holes, which we dubbed the particle-hole Halperin state, has all the properties seen in the experiment: a zero Hall conductivity accompanied by a fractional conductance at the edge, which is one-half of the classic time-reversal invariant topological insulator proposed by Kane and Mele. This state, however, breaks spontaneously time reversal symmetry. Subsequent recent experiments have indeed observed that the state breaks time-reversal symmetry, adding fresh support to the relevance of our theoretical proposal.

Collaborations

- Johannes Deiglmayr, Felix Bloch Institute, University of Leipzig, Germany.
- Justin Song, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore.
- Falko Pientka, Goethe-Universität Frankfurt, Germany.
- Liang Fu, Department of Physics, Massachusetts Institute of Technology, USA.
- Patrick Lee, Department of Physics, Massachusetts Institute of Technology, USA.
- T. Senthil, Department of Physics, Massachusetts Institute of Technology, USA.
- Jun Yong Khoo, Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore.
- Joseph Falson, Department of Applied Physics and Materials Science, Caltech, USA.
- Brian Skinner, Ohio State University, USA.
- Yan Sun, Max-Planck Institute for the Physical Chemistry of Solids, Germany.
- Roderich Moessner, Max-Planck Institute for the Physics of Complex Systems, Germany.
- Francesco Piazza, Max-Planck Institute for the Physics of Complex Systems, Germany.
- David Luitz, Max-Planck Institute for the Physics of Complex Systems, Germany.
- Jeroen van den Brink, Leibniz Institute for Solid State Physics, IFW Dresden, Germany.
- Dennis Wawrzik, Leibniz Institute for Solid State Physics, IFW Dresden, Germany.
- Jorge I. Facio, Leibniz Institute for Solid State Physics, IFW Dresden, Germany.
- Jhih-Shih You, National Taiwan Normal University, Taiwan.
- Po-Yao Chang, National Tsing Hua University, Taiwan.
- Zheng Zhu, Department of Physics, Massachusetts Institute of Technology, USA.
- Debanjan Chowdhury, Department of Physics, Cornell University, USA.
- Donna Sheng, Department of Physics and Astronomy, California State University, USA.
- Thierry Jolicoeur, Laboratoire de Physique Theorique et Modeles statistiques, CNRS, Universite Paris-Sud, Universite Paris-Saclay, Orsay, France.
- Csaba Toke, Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary.

1.10 Max Planck Fellow Group

Max Planck Fellow Group: Dissipative Quantum Matter
(Head: Prof. Jan Carl Budich)

The group has been active since October 2023 on the basis of the Max Planck Fellowship of Prof. Jan Carl Budich (Professor of Quantum Many-Body Theory at TU Dresden) to strengthen the collaboration between TU Dresden and the **mpipks**. The overarching scientific goal of the group is to understand the role of quantum dissipation in the formation, stability, and dynamics of complex ordering patterns, prominently including topological order. In the subsequent paragraphs, we will give a brief overview of the concrete directions explored by the Dissipative Quantum Matter group.

Non-Hermitian Topology. Effective non-Hermitian Hamiltonians have become a widely used tool to account for dissipative effects in a conceptually simple manner, with applications ranging from mechanical and optical meta-materials to correlated electron systems. Recently, the non-Hermitian Hamiltonian approach has been combined with the paradigm of topological matter, thus revealing profound consequences for both the topological classification of matter itself and physical phenomena tied to specific topological properties. Our current focus of interest within this broader field is on non-Hermitian topological properties emerging in quantum many-body systems that are exposed to some sources of decoherence or dissipation, e.g. considering inter-particle scattering as an intrinsic source of dissipation for quasi-particle excitations. Our research objectives range from identifying and predicting novel topological phenomena that have no direct counterpart in coherent (or Hermitian) systems to searching for candidate material systems to realize and functionalize such phenomena in specific material systems. A specific example of our efforts in this field is the study of the spectral sensitivity of non-Hermitian matrices that generically occurs in topologically non-trivial systems, and may be beneficial for enhancing the precision of quantum sensors.

Geometry and Topology in Dissipative Dynamics. Open quantum systems are described by a density matrix that undergoes a Liouvillian time evolution rather than being governed by the familiar Schrödinger equation. Motivated by its ubiquitous importance for the understanding of light-matter interaction, we mainly study Lindblad master equations resulting from the Born-Markov approximation of a weak coupling to a bath with negligible memory time (rapidly decaying correlations), typically provided by a continuum of radiation modes. Remarkably, geometric and topological properties are drastically altered in such Lindbladian dissipative settings, both compared to the coherent Schrödinger equation case and at times even compared to the aforementioned effective non-Hermitian Hamiltonian approach that may be seen as an approximation to a master equation neglecting quantum noise. In this light, we are interested not only in the stability of topological phenomena in the inevitable presence of quantum noise but also in potential new properties enabled by the presence of quantum noise. To this end, we investigate both time-dependent phenomena, such as the temporal accumulation of geometric phases, and steady state properties of quantum master equations.

Obstructions to Quantum State Preparation. Our interest in quantum state preparation is based on the following two aspects. First, in the rapidly growing field of quantum simulation, the main bottleneck to scrutinizing complex quantum matter is neither the engineering of system Hamiltonians exhibiting exciting low temperature states such as topologically ordered states, nor the detection of detailed microscopic observables that has been impressively exemplified with the advent of quantum gas microscopes with single site resolution in optical lattices. Instead, preparing low-temperature (as compared to the energy scales of the engineered Hamiltonian) states remains a key challenge in these inherently non-equilibrium systems that cannot be simply cooled by coupling to a cold bath as electronic materials put into a cryostat. Second, fundamental obstructions arising in the dynamical process of quantum state preparation reveal important information about the structure and complexity of the targeted state and the system as a whole. This encompasses topological obstructions to preparing topological states of quantum matter that are separated from any trivial starting point by a quantum phase transition as well as obstructions imposed by computational complexity in the field of adiabatic quantum computing, where the targeted state encodes the solution to a computationally hard problem. Within the broad

field of state preparation, the dissipative quantum matter group focuses on exploring as to what extent dissipation can assist or even facilitate the preparation process, e.g. by harnessing incoherent processes to circumvent quantum phase transitions.

Computational Tools for Dissipative Quantum Many-Body Dynamics. Our group is also active in developing and extending computational methods for studying dissipative quantum many-body dynamics. There, our main expertise is on variational approaches, both in the mostly deterministic context of tensor networks, such as matrix product states (MPS) and in the stochastic framework of variational Monte Carlo methods. A recent effort along these lines combines our analytical experience on geometric phases with MPS methods for the time evolution of mixed quantum states. The latter are typically cast into the MPS framework as purified quantum states, i.e. pure states in an extended Hilbert space. Finding an optimal time-dependent gauge on the auxiliary Hilbert space then becomes a hard problem that largely affects the computational efficiency of the entire approach. Using mixed state geometric phases as a guiding principle to identify such a gauge, we could substantially improve on previous methods addressing the same issue for a wide range of use cases.

Collaborations.

- We have fruitful collaborations within the mpi**pks** with
  - Dr. Marin Bukov on the geometry of periodic driving as well as the potential of counterdiabatic driving for the preparation of quantum many-body states.
  - Dr. Pieter Claeys on the relation between obstructions to quantum state preparation and limitations to finite depth quantum circuits including measurement layers.
- Collaborations with groups outside of mpipks include
  - Prof. Emil J. Bergholtz (Stockholm University, theory) on the topological properties of effective non-Hermitian Bloch Hamiltonians, and the potential of non-Hermitian topological systems for quantum sensing.
  - Prof. Sebastian Diehl (University of Cologne, theory) on the non-equilibrium field theory description of dissipative topological matter.
  - Dr. Joseph Dufouleur (IFW Dresden, experiment) on realizing and further developing topological sensors using the physical platform of multi-terminal transport settings.
  - Prof. Karl Leo (TU Dresden, experiment) On experimentally realizing dissipative topological phenomena in photonic crystals based on organic semiconductor materials, with particular reference to coupled resonator arrays exhibiting spatial patterns of optical gain and loss.
  - Prof. Frank Pollmann (TU Munich, theory) On tensor network approaches for numerically simulating dissipative quantum many-body dynamics, with particular reference to systems encoding the solution to computationally hard problems in their steady states.
  - Prof. Giorgio Sangiovanni (University of Würzburg, theory) on the emergence of effective non-Hermitian Hamiltonians in correlated quantum materials, in particular using the framework of dynamical mean field theory (DMFT).

1.11 Advanced Study Groups

Advanced Study Group 2019/2022: Open quantum systems far from equilibrium
(Convenor: Prof. Dr. Dr. h.c. mult. Peter Hänggi, University of Augsburg, Germany)

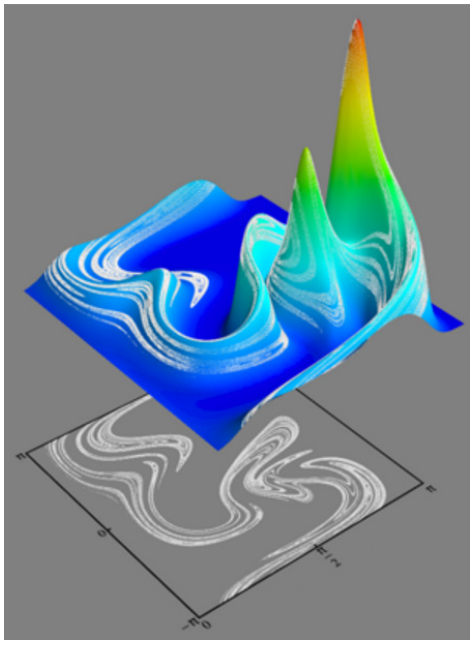
Objectives and Focus. The goal of this Advanced Study Group (ASG) was to explore open many-body quantum systems far from equilibrium. This effort intersects active fields like quantum thermodynamics, computational quantum physics, and the physics of open quantum systems. Particular emphasis was placed on investigating Dissipative Quantum Chaos, quantum attractors, and transport phenomena in strongly interacting quantum systems.

Timeline and Members. The ASG progressed through three stages:

1. December 2019 – January 2020
2. June – August 2021
3. December 2021 – February 2022

The core team included convenor Prof. Peter Hänggi (University of Augsburg, Germany) and Prof. Sergiy Denisov (Oslo Metropolitan University) and Prof. Dario Poletti (Singapore University of Technology and Design). The group hosted visitors such as Prof. Dariusz Chruściński (Nicolas Copernicus University), Prof. Karol Życzkowski (Jagiellonian University), and Dr. Juzar Thingna (Institute for Basic Science, South Korea). **mpipks** members, including Prof. David Luitz (at the time leader of the group "Computational Quantum Many-body Physics", now professor at the Institute of Physics, University of Bonn), Prof. Francesco Piazza (at the time leader of the group "Strongly Correlated Light-Matter Systems", now professor at the Department of Theoretical Physics I, University of Augsburg), and Prof. Ivan Khaymovich (at the time staff scientist at the **mpipks** Condensed Matter Division, now assistant professor at NORDITA, Stockholm, Sweden). Last but not least, researchers from TU Dresden participated in the group discussions, including Prof. Carsten Timm (Chair of Theory of Condensed Matter).

Key Topics addressed by the ASG. Dissipative Quantum Chaos; Spectral properties of random generators of Markovian evolution (both quantum and classical); Development of such concepts of "superdecoherence" and "coherefication" of Markovian generators; Quantum Lyapunov exponents; Open Floquet Systems; Time-periodic Lindblad equations; and Transport in Open strongly-interacting Many-Body Systems.



Example of a many body quantum system far from equilibrium we depict here the Quantum attractor (colored) versus its classical attractor (white dots); Figure adapted from Ref. [1].

Main Objectives of the ASG. In some further detail the ultimate goal of the ASG has been to explore the role of dissipation in complex (many-body) quantum systems such as the concept of quantum attractors; i.e., strongly non-equilibrium asymptotic states of open quantum dissipative systems, subjected to (controllable) dissipation and alike the consequences for the dynamics when time-periodically perturbations are applied. A particularly challenging theme of the ASG-group was to investigate manifestations of Dissipative Quantum Chaos, i.e., phenomena emerging in the dynamics of open quantum systems that operate far out of thermal equilibrium.

Particularly, a prime goal of the group was to investigate manifestations of Dissipative Quantum Chaos occurring in the dynamics of many-body open quantum systems when shifted far out of equilibrium. The existing well-developed theory of Quantum Chaos addresses exclusively Hamiltonian systems; i.e., those that are being fully isolated from the influence of their environments. The corresponding theoretical predictions have been tested and validated, by use of either microwave billiards, ultra-cold atoms or stylized quantum electronic circuits, to name but a few. However, with the emergence of new types of real-life quantum systems, such as optomechanical systems, microwave superconductive circuits, and polaritonic devices, the Hamiltonian idealization lost much of its appeal. In particular, the omnipresent impact of dissipation in these systems generates a full-fledged generator of time-evolution, no less complex and diverse than the unitary evolution generated by quantum Hamiltonians. Consequently, this situation calls for the challenge to delve into the presumably rich and promising new physics this very type of complex quantum evolution may disclose.

Particularly, the ASG addressed the following challenges:

- What are the spectral signatures of Dissipative Quantum Chaos?
- Open (driven) Floquet systems: do there exist effective time-independent Lindbladians?
- The Loschmidt echo in Luttinger liquids after a spatially homogeneous and inhomogeneous interactions quench: in spite of the non-equilibrium nature of the problem, the Luttinger model still describes reasonably well the short and long time dynamics in the XXZ Heisenberg chain, studied numerically using matrix product state based methods.
- Quantum thermodynamics: How to measure transport of mass and charge in open many-body systems far from equilibrium and, above all, how to quantify physical quantities such as quantum "work" and "heat" which formally cannot be encoded in terms of quantum observables (but rather constitute quantum processes).

[1] M. Hartmann, D. Poletti, M. Ivanchenko, S. Denisov, P. Hänggi, New J. Phys. **19(8)** (2017) 083011.

Advanced Study Group 2024/2025: Strongly Correlated Extreme Fluctuations
(Convenor: Prof. Abbas Ali Saberi)

The Advanced Study Group (ASG) explores the timely and transformative interplay of two pivotal concepts: *strong correlations* and *extreme fluctuations*. This interaction often gives rise to emergent phenomena and novel observations that transcend disciplinary boundaries. By uncovering universal principles governing complex systems, this interplay inspires groundbreaking research across diverse fields, including physics, climate science, and beyond [1–3].

To reflect the interdisciplinary nature of this ASG, we have brought together leading researchers from distinct fields who not only represent diverse disciplines but also embody the essence of the ASG's title. The core members—Mehran Kardar (MIT, USA), Jürgen Kurths (PIK, Germany), and Martin Zirnbauer (University of Cologne, Germany)—bring expertise in statistical physics, climate dynamics, and condensed matter physics, respectively. The ASG is structured into three subgroups, each led by one of these pioneers to address the complexity and breadth of the topic.

The ASG began its mission in July 2024, with the core members initiating collaborative research projects at the Max Planck Institute for the Physics of Complex Systems (mpi**pks**). These projects involve interactive engagement with various research groups, including postdoctoral fellows and resident researchers. Esteemed visiting scientists such as Constantino Tsallis (Santa Fe Institute, USA) and Satya Majumdar (Université Paris-Saclay, France) have further enriched these efforts, contributing to the development of innovative research collaborations alongside mpi**pks** members like Roderich Moessner (Director), Holger Kantz (Head of the Nonlinear Dynamics and Time Series Analysis group), Fatemeh Aghaei (Postdoc), and Sen Mu (Postdoc).

In 2025, the ASG plans to host additional distinguished visitors, including Gernot Akemann (University of Bielefeld, Germany), Mehrnaz Anvari (Fraunhofer ISCAI, Germany), Hugues Chaté (CEA-Saclay, France), Thomas Guhr (University of Duisburg-Essen, Germany), Hans Herrmann (CNRS, France), Matteo Marsili (ICTP, Italy), Muhammad Sahimi (USC, USA), Attilio Stella (University of Padova, Italy), Martin Weigel (Technische Universität Chemnitz, Germany), and Robert M. Ziff (University of Michigan, USA).

The ASG is structured around several key research directions, including:

- Spectral properties of random matrices with strongly interacting elements and the statistics of their extremes.
- Universal dynamics of percolation models on complex networks, incorporating triadic interactions.
- Spectral analysis of critical atmospheric variables to uncover universal scaling laws in eigenvalue spectra.
- Statistical properties of directed polymers in random media (DPRM) using the six-vertex model, focusing on the transition between edge and bulk behaviors in eigenvalue spectra.
- Multifractal properties of critical wave functions and universal features at the plateau transition of the integer quantum Hall effect.

Through its interdisciplinary approach, collaborative framework, and engagement with leading experts, the ASG aims to advance the understanding of the universal mechanisms underlying strongly correlated extreme fluctuations and their far-reaching applications.

Awards of people in the group:

- Mehran Kardar (Core member): Boltzmann medal 2025

[1] Kardar, M., Parisi, G., Zhang, Y.-C. *Dynamic scaling of growing interfaces*. Phys. Rev. Lett. **56**, 889–892 (1986).

[2] Majumdar, S. N., Comtet, A. *Extreme value statistics and random matrix theory*. J. Stat. Mech. **2005**, P06004 (2005).

[3] Albeverio, S., Jentsch, V., Kantz, H. *Extreme Events in Nature and Society*. Springer (2006).

Chapter 2

Selection of Research Results

2.1 Long-lived solitons and their signatures in the classical Heisenberg chain

ADAM MCROBERTS AND RODERICH MOESSNER

Introduction Motivated by the KPZ scaling recently observed [1] in perhaps the simplest many-body spin system – the classical ferromagnetic Heisenberg chain – we investigate the role of solitonic excitations in this model. We find that the Heisenberg chain, although well-known to be non-integrable, supports a two-parameter family of long-lived solitons [2] . We explicitly construct infinitely long-lived stationary solitons, and provide a construction for moving solitons. The lifetime t^* of these solitons grows very rapidly: at low temperature, we find $t^* \sim T^{-\zeta}$ with an exponent possibly as large as $\zeta = 8$. This can render the crossover to ordinary diffusion practically inaccessible [3].

Model and its one-soliton solutions The classical Heisenberg chain Hamiltonian is

$$\mathcal{H} = -J \sum_i (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - 1), \tag{1}$$

where $\mathbf{S}_i$ are classical $O(3)$ vectors at sites i, with nearest-neighbour ferromagnetic interaction strength J.

We first provide exact (though not closed-form) expressions for stationary solitons in the form of an (implicit) solution to the non-linear equations of motion of the Heisenberg model. For this, we use canonical coordinates, $z_i = S_i^z$, $\phi_i = \arctan(S_i^y/S_i^x)$. Our ansatz is based on (i) stationarity of the z-components, i.e., $\dot{z}_i = 0, \forall i$, (ii) spatially uniform azimuthal angles ϕ_i (except for a discontinuity of π across the centre), and (iii) a uniform rotation frequency of the in-plane spin-components, i.e., $\phi_i(t) = \phi_i(0) + \omega t, \ \forall i$. This ansatz reduces the equations of motion to consistency equations for the z_i, which, for a chosen frequency ω, may be solved numerically to arbitrary precision:

$$\begin{aligned}\dot{\phi}_i = \omega =& J \frac{z_i}{\sqrt{1-z_i^2}} \left(\sqrt{1-z_{i+1}^2} + \sqrt{1-z_{i-1}^2} \right) \\ & - J\,(z_{i+1} + z_{i-1})\,.\end{aligned} \tag{2}$$

This yields stable stationary solitons containing spins deviating from full polarisation across an arbitrary width $\sim 1/R$. This constitutes the first (to our knowledge) exact soliton in the Heisenberg model. We also note that this construction extends more generally to 1D spin chains.

Moving solitons To construct a moving soliton, we consider objects for which (i) there is, for all times, a unique local minimum of $z_i(t)$; (ii) the unique local minimum propagates with a constant velocity, and (iii) for $t > t_A$, the torsion $\tau = \sum_i \tau_i$ is constant in time:

$$\tau_i = \frac{\boldsymbol{S}_i \cdot (\boldsymbol{S}_{i+1} \times \boldsymbol{S}_{i-1})}{(1 + \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})(1 + \boldsymbol{S}_i \cdot \boldsymbol{S}_{i-1})}\,. \tag{3}$$

We thus find solitons covering a remarkably large range sizes (R) and velocities ($\sim k$). We find no indication of a finite lifetime of these single soliton states. Moreover, the torsion is otherwise generally not a conserved quantity of the Heisenberg chain, but it is conserved in these states, up to numerical accuracy.

While stationary solutions of non-linear classical equations of motion are well known, stable moving solitons are not expected to exist in a generic system. From this perspective, our finding of propagating objects with apparently unlimited stability is remarkable.

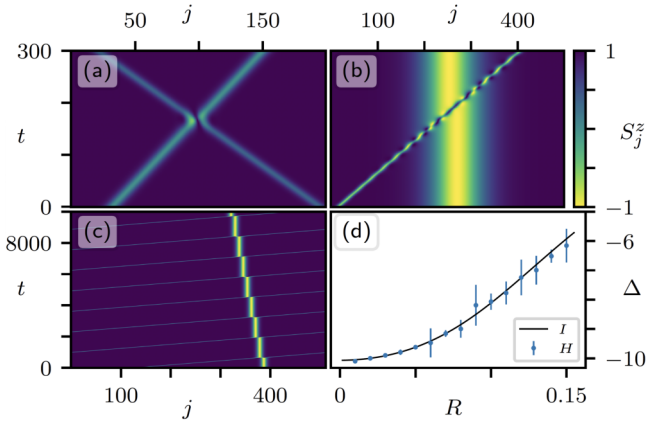


Figure 1: Soliton scattering in the Heisenberg chain. Colour-scale shows the z-components, and is the same for (a), (b), and (c). (a) Single scattering event between two solitons with parameters $(R, k) = (0.1, 0.1)$ and $(R', k') = (0.1, -0.15)$. (b) Screening of the magnetisation transported by a narrower soliton as it moves through a wider soliton. (c) Repeated scattering of two solitons $[(R, k) = (0.1, 0.1)$ and $(R', k') = (0.1, 0)]$ under periodic boundary conditions. (d) Comparison of the scattering phase-shift $\Delta(R, k = 0; 0.1, 0.1)$ in the Ishimori chain (solid line) and in the Heisenberg chain, for stationary target solitons. Phase-shifts in the Heisenberg chain obtained by averaging over 10 scattering events, cf. (c), and over the relative phases of the solitons – the error bars are the standard deviation w.r.t. the relative phases.

Two-soliton scattering We now turn to interactions between the solitons. To set the stage, we briefly recall scattering in the Ishimori chain, an exactly integrable spin chain with an interaction $\sim J \sum_i \log[1 + \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}]$ replacing the Heisenberg interaction. As a fully integrable model, interactions are completely described by the two-soliton phase-shifts, even for thermal multi-soliton states. When two solitons collide, the asymptotic result (compared to two separate one-soliton solutions) is unchanged, except that the solitons are displaced by a so-called phase-shift depending on their velocities v

$$\begin{aligned}\Delta(R, k; R', k') &= \operatorname{sgn}(v(R, k) - v(R', k')) \\ &\times \frac{1}{2R} \log \left[\frac{\cosh(2(R + R')) - \cos(2(k - k'))}{\cosh(2(R - R')) - \cos(2(k - k'))} \right]\end{aligned} \tag{4}$$

experienced by the soliton (R, k), due to a collision with the soliton (R', k').

Fig. 1 displays the scattering of two Heisenberg solitons. The solitons survive scattering essentially unchanged, Fig. 1(a), akin to the fully integrable model. While the collisions do leave the solitons unchanged asymptotically, the magnetisation of a moving soliton is 'screened' during the collision with a larger soliton as seen in Fig. 1(b). Importantly, solitons actually survive multiple collisions, Fig. 1(c), with the change to their trajectories apparently given by simple consecutive phase-shifts.

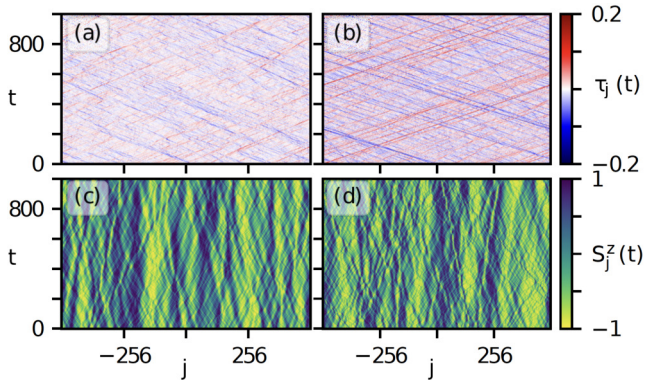


Figure 2: Solitons in the thermal state at $T = 0.1J$ for the Heisenberg (left) and integrable Ishimori (right) chains. Upper and lower panels show torsion $\tau_j(t)$, and $S^z_j(t)$ respectively. Ballistic trajectories are clearly visible in the torsion plots. These ballistic trajectories can also be seen in the plots of S^z, where the magnetisation carried by a soliton changes as it moves through the chain – the mechanism replacing ballistic with KPZ spin transport.

KPZ regime Having established the existence and nature of the almost integrable behaviour of the Heisenberg chain, we now address the KPZ scaling observed at low temperatures [1]. In integrable chains, KPZ – rather than ballistic – spin transport emerges as follows. As smaller, faster solitons move through larger, slower solitons, they rotate to the 'local vacuum' within the larger soliton. Thus, in any thermal state, the magnetisation carried by the smaller solitons is screened on a timescale set by the rate at which they encounter larger solitons. Since long-lived solitons are also present in the classical Heisenberg chain at low temperature, this provides a qualitative picture of and explanation for the KPZ regime in spin transport. A comparison between the time evolution of states with a finite energy (and hence soliton) density is shown in Fig. 2.

Absent integrability, scattering in the Heisenberg chain is not expected to be perfectly lossless. Indeed, there is a very small amount of radiation emitted during the collision (approx. $\delta S^z \sim 10^{-6}$ in magnitude) in Fig. 1(a). Second, scattering from narrow solitons at small k (where solitons with a wider range of the parameter R exist) can emit significant amounts of radiation, although, curiously, the modified solitons that emerge appear to be stable to subsequent collisions. Also, the velocities of the solitons remain unaffected by the collisions.

Crossover to ordinary diffusion The question then naturally arises how non-integrability will assert itself in generating diffusive, rather than KPZ, long-time behaviour. This forms part of the broader question of how stable 'non-generic' behaviour in many-body systems can be in practise. Crucially, since this crossover is non-universal – it concerns the *establishment* of hydrodynamics – extracting a parametrisation requires a concrete model for the processes driving it. This analysis is somewhat involved and extracting the resulting parameters is numerically challenging. The resulting picture, however, is simply summarised [3]: the crossover from KPZ-like superdiffusion to ordinary diffusion occurs on a crossover timescale which depends on temperature T algebraically with a very high exponent α:

$$t^* \sim T^{-\zeta}\,, \quad \zeta \approx 8\,. \tag{5}$$

However, the low-T dynamics is, in fact, richer than the crossover purely from KPZ-like superdiffusion to asymptotic ordinary diffusion. First, an initial ballistic regime becomes increasingly long-lived as T is lowered: the density of solitons decreases, which implies an increase in the timescale each soliton contributes ballistically to spin transport. Second, besides the KPZ-like and diffusive regimes, the availability of the decay channel involving solitons of different sizes favours a regime of logarithmically-enhanced diffusion between these two. There is, at present, no theory providing sufficient quantitative guidance to allow fits distinguishing between these different scenarios, and, in any case, one would require well-separated timescales and hence a huge simulation/experimental time window, to properly resolve these and their crossovers. Indeed, we estimate that at $T = \infty$, both decay channels make comparable contributions to the diffusion constant, so that this competition will likely persist to finite T.

We reiterate that the Heisenberg chain we have considered has not been especially chosen for the purpose of obtaining long-lived superdiffusive regimes; that this happens in, arguably, one of the simplest many-body models makes it all the more remarkable that anomalous hydrodynamics can persist over such enormous timescales.

[1] A. J. McRoberts, Thomas Bilitewski, Masudul Haque, Roderich Moessner, *Anomalous Dynamics and Equilibration in the Classical Heisenberg Chain*, Phys. Rev. B **105**, L100403 (2022).

[2] A. J. McRoberts, Thomas Bilitewski, Masudul Haque, Roderich Moessner, *Long-lived Solitons and Their Signatures in the Classical Heisenberg Chain*, Phys. Rev. E **106**, L062202 (2022).

[3] A. J. McRoberts, Roderich Moessner, *Parametrically long lifetime of superdiffusion in non-integrable spin chain*, Phys. Rev. Lett. 133, 256301 (2024).

2.2 Non-Hermitian delocalization in 1D via emergent compactness

LIANG-HONG MO, RODERICH MOESSNER, AND HONGZHENG ZHAO

Summary Potential disorder in 1D leads to Anderson localization of the entire spectrum. How can this localisation be circumvented? We find that this is possible by sacrificing Hermiticity via adding *imaginary* potential disorder [1]. While an entirely random potential generally still leads to localization, imposing minimal spatial structure to the disorder can yield delocalization: it endows the concomitant transfer matrix with an $\mathrm{SU}(2)$ structure, whose compactness in turn translates into an infinite localization length. The fraction of delocalized states can be tuned by the choice of boundary conditions. This result thus identifies a new mechanism for delocalisation, and in doing so it highlights the role of *structured* disorder in the genesis of new phenomena, in keeping with our investigations which have led to the identification of partial spatiotemporal forms of order [2].

Concretely, we present a model which shows that 1D delocalized eigenstates can be realized by purely on-site energy gain and loss, without sacrificing reciprocity and spatial randomness. This also allows us to identify analytically tractable mobility edges. The key ingredient involves imposing a minimal structure on a binary potential, which we dub "dipolar disorder". The corresponding transfer matrix generally belongs to the non-compact $\mathrm{SL}(2,\mathbb{C})$ group; hence, a random product of such matrices leads to a positive Lyapunov exponent, i.e., a finite localization length. However, the possible existence of an emergent compact $\mathrm{SU}(2)$ structure, which we identify, in the transfer matrix for the real-valued spectrum results in a zero Lyapunov exponent. It, in turn, leads to an infinite localization length, protecting delocalization against disorder. This $\mathrm{SU}(2)$ structure can be revealed by a simple analytical procedure, cf. Fig. 1(a), allowing the exact determination of a mobility edge, for which the usual numerical approach faces difficulties, especially in the thermodynamic limit.

Model The Schrödinger equation for 1D tight-binding Hamiltonian H with uniform and reciprocal nearest-neighbor hopping and on-site potential V_j reads

$$E\Psi_j = \Psi_{j+1} + \Psi_{j-1} + V_j\Psi_j, \quad j \in \mathbb{Z}, \tag{1}$$

where $\Psi_j \equiv \langle j|\Psi\rangle$ is the real-space wavefunction on site j and E defines the energy. It can be rewritten as

$$\begin{pmatrix}\Psi_{j+1}\\ \Psi_j\end{pmatrix} = T_j\begin{pmatrix}\Psi_j\\ \Psi_{j-1}\end{pmatrix},\ T_j = \begin{pmatrix}E-V_j & -1\\ 1 & 0\end{pmatrix}, \tag{2}$$

where T_j is the transfer matrix. For the entire chain with length N, the transfer matrix reads $T_{\mathrm{tot}}^{(N)}=\prod_{j=1}^{N} T_j$. The corresponding Lyapunov exponent λ_L is defined as $\lambda_L \equiv \lim_{N\to\infty} \log||T_{\mathrm{tot}}^{(N)}||/N$, where $||...||$ denotes the 2-norm. For a given eigen-energy E, the localization length $\xi(E)$ can be obtained as the inverse of the Lyapunov exponent λ_L of $T_{\mathrm{tot}}^{(N)}$. In the conventional Hermitian Anderson model where V_j is a real random variable, λ_L is positive for any energy E in 1D, so that all eigenstates are localized.

We consider an *imaginary* binary random potential, i.e., $V_j{=}i\,c_j\,V$, with $c_j \in \{-1,+1\}$ and $V{\in}\mathbb{R}$. We focus on states with real energies and obtain transfer matrices

$$T_\pm = \begin{pmatrix}E \pm iV & -1\\ 1 & 0\end{pmatrix}, \tag{3}$$

which satisfy $T_+ = T_-^*$ and belong to the group $\mathrm{SL}(2,\mathbb{C})$. Its associated manifold is non-compact. According to Furstenberg's theorem, in a non-compact manifold, a random product of matrices generally leads to a positive Lyapunov exponent. Therefore, just as the conventional Hermitian Anderson model, the onsite imaginary potential can localize all eigenstates.

Emergent compactness We impose a dipolar structure into the spatial disorder, such that the minimal building block of the disorder becomes either $\{iV,-iV\}$, or $\{-iV,iV\}$. Each block has a balanced energy gain (iV) and loss ($-iV$), resulting in a parity-time symmetry within the block, also referred to as "local parity-time symmetry". By contrast, global parity-time symmetry is absent due to the spatial randomness of the blocks. The corresponding transfer matrices for two consecutive sites become $\mathcal{M}{=}T_+T_-$, $\mathcal{N}{=}T_-T_+$, which satisfy $\mathcal{M}=\mathcal{N}^*$ and exhibit a real trace.

A peculiar feature appears in this dipolar construction: as schematically illustrated in Fig. 1(a), an emergent compactness arises because both $\mathcal{M}$ and $\mathcal{N}$ can simultaneously be transformed into $\mathrm{SU}(2)$ matrices via a similarity transformation. As the corresponding manifold for the $\mathrm{SU}(2)$ group is compact, the Lyapunov exponent for a series of random multiplication of $\mathcal{M}$ and $\mathcal{N}$ vanishes.

A subset of real eigenenergies allows for such a similarity transformation and the crucial ingredient is simply:

$$\mathrm{Tr}\,(\mathcal{M}\mathcal{N}) \le 2. \tag{4}$$

This, together with the condition $\mathcal{M}=\mathcal{N}^*$, guarantees that the eigenvalues of both $\mathcal{M}$ and $\mathcal{N}$ satisfy the spectral requirements of the $\mathrm{SU}(2)$ group. Numerically, one can efficiently scan over the entire parameter space and show that Eq. 4 leads to the blue region in Fig. 1(b), including the black line–the analytical expression for the mobility edge is $-4E^2+E^4+2E^2V^2+V^4=0$.

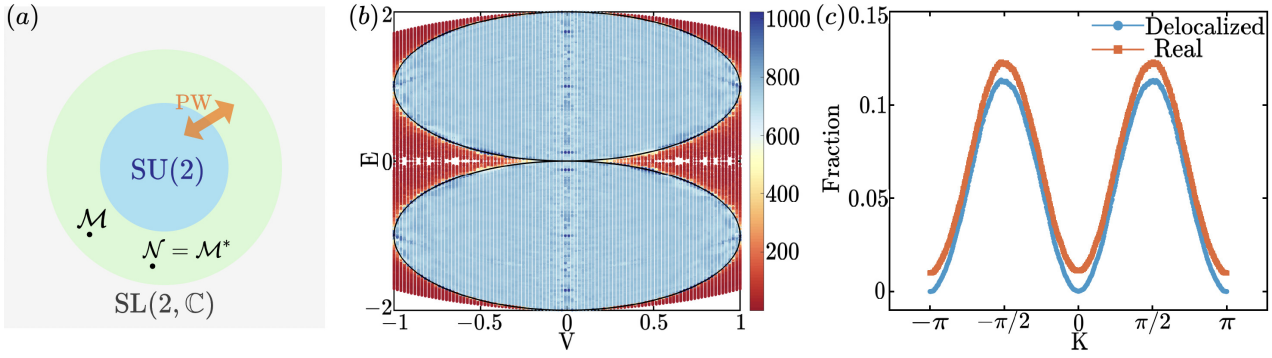


Figure 1: (a) Schematic for the emergent compact structure. The overall gray region denotes the non-compact $\mathrm{SL}(2,\mathbb{C})$ group, which contains the compact $\mathrm{SU}(2)$ structure (blue). The green region denotes a subset of $\mathrm{SL}(2,\mathbb{C})$, inside which a matrix element as well as its conjugation can be simultaneously mapped to $\mathrm{SU}(2)$ matrices, via a similarity transformation denoted PW. The dipolar transfer matrices, $\mathcal{M}$ and $\mathcal{N}$, belong to this subset and hence a random product of the two leads to zero Lyapunov exponent. (b) Participation ratio calculated for each eigenstate at different real energies E and disorder strength V. The emergent compactness leads to delocalized eigenstates (blue), separated from the localized states (red) by an exact mobility edge (black). This black line is obtained by analyzing the possible existence of a similarity transformation. In numerical simulation, we scan over all possible boundary conditions with a twisted angle K and sample different realizations of the disorder potential. (c) By tuning K, we can control the fraction of real energies (orange) in the entire spectrum and the delocalized eigenstates therein (blue). For periodic and anti-periodic boundary conditions $K{=}0,\pi$, the fraction of eigenstates is around 10^{-4}, a small but nonzero value. Yet, for other K values, most real energies are delocalized. For numerical simulation, we use $V = 0.3, 2L = 1024$.

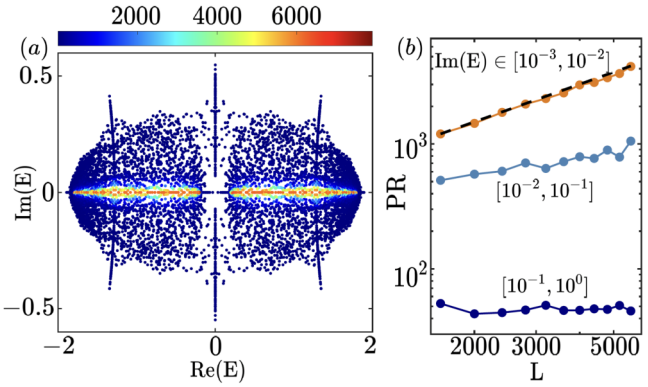


Figure 2: (a) Participation ratio for the entire complex spectrum. Our simulations use $V = 0.6$, $K = \pi/2$ and system size $L = 8192$. Most eigenstates with complex energies are localized, while a small fraction of energies near the real axis (bright region) exhibit a large PR, suggesting delocalization. (b) System size scaling of PR, averaged over eigenstates within different imaginary energy windows. The real part of the energy is fixed within the range $[0.8, 1.2]$. For an eigenvalue sufficiently close to the real axis, PR exhibits linear (black dashed line) scaling in L.

Consequently, inside the blue region in Fig. 1(b), the dipolar transfer matrices have an emergent compact $\mathrm{SU}(2)$ structure, i.e. a vanishing Lyapunov exponent and a diverging localization length. In contrast, localisation occurs for parameters in the red region. There, both $\mathcal{M}$ and $\mathcal{N}$ have an eigenvalue larger than one, thus they do not belong to any compact subgroup of $\mathrm{SL}(2,\mathbb{C})$.

Complex spectrum For complex energies, the emergent $\mathrm{SU}(2)$ structure is not guaranteed, nor is the existence of a delocalized eigenstate. In fact, most of the complex spectrum becomes localized, as shown in Fig. 2 (a).For eigenvalues close to the real axis, matrix elements of $T_\pm$ (Eq. 3) are still dominated by the real part of the energy. Therefore, the localization length can still be large, even comparable to system sizes that are numerically accessible. Indeed, as shown in Fig. 2 (a), a bright region with large PR values appears, indicating the possible existence of delocalized eigenstates.

Discussion While focusing on the eigenstate properties of the system, we emphasize that this emergent compact structure can also lead to interesting dynamical phenomena that may not exist in non-Hermitian systems with an entirely localized spectrum.

There are various experimental platforms capable of realizing tunable control over the on-site gain and loss, such as photonic waveguides and mechanical systems. Therefore, the proposed dipolar potential structure, as well as the predicted delocalization should be readily accessible in these physical settings.

Finally, we emphasize that, due to the broad applicability of the transfer matrix method, the emergent compactness could have significant implications at a more general level, particularly in many-body systems. For instance, a similar transfer matrix method has been developed in the study of dual unitary and Gaussian quantum circuits, as well as within the framework of time-dependent driven systems exhibiting conformal symmetry. We anticipate that this emergent compactness will lead to more surprises and unexpected dynamical non-equilibrium many-body phenomena.

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2.3 Quantum information scrambling in unitary circuit dynamics

MICHAEL A. RAMPP, RODERICH MOESSNER, AND PIETER W. CLAEYS

Introduction. The dynamical behaviour of strongly correlated quantum many-body systems out of equilibrium is notoriously hard to describe. Quantum many-body dynamics is intimately related to questions of thermalization, information scrambling, quantum chaos, and hydrodynamics, yet tractable models of many-body dynamics remain scarce. In recent years, unitary circuits have gained increased attention as minimal models for quantum many-body dynamics in which these questions can be tackled. A unitary circuit describes a sequence of unitary transformations–or gates–each acting on local degrees of freedom (qubits or spins). This dynamics reproduces both the locality and unitarity inherent in generic lattice dynamics. On the experimental side, such circuits are naturally realized within the gate-based paradigm of quantum computing. On the theoretical side, the framework of random circuits presents a valuable analytical tool: Averaging over random circuit realizations can be used to map complicated problems of quantum dynamics to tractable problems of statistical mechanics.

In the absence of randomness, exact results for chaotic circuit dynamics are limited to so-called dual-unitary circuits. These models are characterized by a space-time duality that allows a variety of dynamical quantities to be analytically characterized. Solvability however comes at a cost in genericity, and in several respects dual-unitary circuits display behaviour that differs strikingly from the phenomenology observed numerically in more generic models. Effective theories for generic structured circuits are hence required. In Ref. [1], dual-unitary circuits were used as the starting point to develop a perturbation theory for the operator dynamics in circuits 'close' to dual-unitarity, studying whether, and how, small deviations from dual unitarity recover fully generic many-body dynamics. These results allow for an efficient numerical evaluation of the operator dynamics and present a clear intuitive picture for the mechanism of information scrambling.

Model. We consider unitary evolution described by a "brick wall" quantum circuit as illustrated in Fig. 1(a). Denoting the time evolution operator as $\mathcal{U}(t)$, we write $\sigma_\alpha(x,t) = \mathcal{U}(t)^\dagger \sigma_\alpha(x) \mathcal{U}(t)$ as the time-evolved Pauli operator $\sigma_\alpha(x)$ on site x and consider the so-called *out-of-time-order correlator* (OTOC):

$$C(x,t) = \langle \sigma_\alpha(0,t)\sigma_\beta(x,0)\sigma_\alpha(0,t)\sigma_\beta(x,0)\rangle, \qquad (1)$$

with respect to the maximally mixed state, $\langle O\rangle \equiv \mathrm{tr}[O]/\,\mathrm{tr}[\mathbf{1}]$. This function quantifies the spreading of operators and the scrambling of information into non-local degrees of freedom and is experimentally accessible in (digital) quantum simulation platforms. In random circuits the OTOC front undergoes a biased random walk [2]. The resulting propagation speed is called the *butterfly velocity* v_B and sets the maximal speed at which information can spread. For dual-unitary circuits space-time duality implies that the OTOC propagates with maximal butterfly velocity, $v_B = 1$, as theoretically predicted in Ref. [3] and experimentally observed in Google Quantum AI's quantum simulator [4].

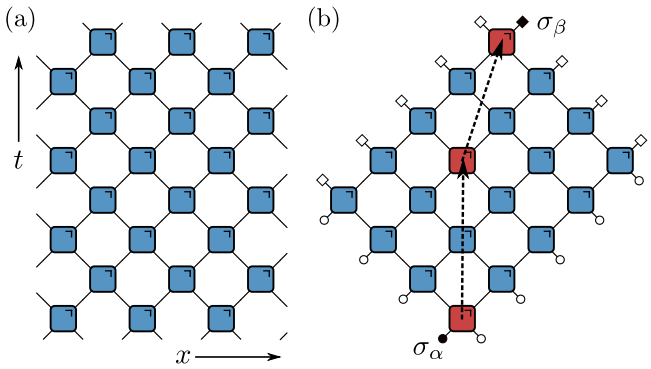

Figure 1: (a) A "brick wall" quantum circuit. The quantum degrees of freedom are arranged in a horizontal row with two-site unitary gates acting alternately on the even and odd links between them. Discrete time runs vertically. (b) Graphical depiction of processes contributing to the OTOC. When dual unitarity is broken, the OTOC front can scatter into the light cone and the OTOC is given by a weighted sum over all paths. Dual-unitary gates are depicted in blue and dual-unitarity-breaking gates in red.

Approach. A full calculation of the OTOC is exponentially costly. From unitarity the calculation of the OTOC can be reduced to the contraction of a tensor network of the form in Fig. 1(b), which can in turn be understood as the contraction of powers of a transfer matrix along the diagonal ("light-cone") direction. In the dual-unitary case, powers of this transfer matrix can at late times be replaced by a projector on its leading eigenspace, the so-called maximally chaotic subspace (MCS). This maximally chaotic subspace encodes a perfect transfer of quantum information, and results in an OTOC for dual-unitary circuits in which the front propagates with $v_B = 1$. For more general circuits, we project the transfer matrix to the MCS, similar in spirit to degenerate perturbation theory, and compute the OTOC with the projected transfer matrix. This approach presents both a numerical advantage, reducing the exponential cost of calculating the OTOC to a polynomial one, and an analytical advantage since, in this projected space, the OTOC allows for a systematic expansion in terms of tractable scattering paths. The ma-

trix elements of this transfer matrix can additionally be given a quantum-information theoretic interpretation.

Results. The resulting OTOC for a representative circuit away from dual-unitarity is shown in Fig. 2, exhibiting the expected ballistic propagation with a non-maximal butterfly velocity $v_B < 1$ and diffusive broadening with time. From the structure of the transfer matrix it follows that the full OTOC can be evaluated as a summation over possible scattering paths, leading to a discrete path integral. Further analytical insight can be obtained by restricting this summation over paths. Restricting to paths in which single steps are at most of size 1, the discrete path integral can be explicitly evaluated. An asymptotic expansion yields a front that takes the form

$$C(x,t) \approx \frac{1}{2}\left(1 + \mathrm{erf}\left(\frac{x - v_B t}{\sqrt{2Dt}}\right)\right), \tag{2}$$

describing ballistic propagation with butterfly velocity $v_B = (1 - z_1)/(1 + z_1)$ and diffusive broadening with diffusion constant $D = v_B(1 - v_B^2)$. Here $z_1 = 1 - [q^2/(q^2 - 1)]E(U)$, where q is the dimension of the local Hilbert space and $E(U)$ is the linear operator entropy of the local gates in the circuits. This operator entropy fixes $0 \leq z_1 \leq 1$, with $z_1 = 0$ if and only if the circuit is dual-unitary. It can be shown that higher-order paths are suppressed and only serve to renormalize the butterfly velocity and diffusion constant, consistent with Fig. 2. Including paths in which single steps are at most of size 2, the profile is modified to

$$C(x,t) \to C\left(x + \frac{t-x}{2}\xi, t - \frac{t-x}{2}\xi\right), \tag{3}$$

with $\xi = z_2/(q^2 z_1)$, where z_2 is defined as z_1 but for two diagonally composed gates. This result can be understood by noting that the path integral is asymptotically dominated by the typical path. If $z_2 \ll z_1$, the typical fraction of steps of size two is approximately given by the ratio of scattering amplitudes $\xi = z_2/(q^2 z_1)$, shifting the operator front into the light cone.

This path-integral interpretation extends the biased random walk picture of random circuits by including the dependence on the choice of unitary gates. No scattering is allowed in the dual-unitary limit, resulting in purely ballistic propagation of the OTOC with maximal velocity, while deviations from dual unitarity allow for scattering, with scattering amplitudes set by the operator entanglement entropies.

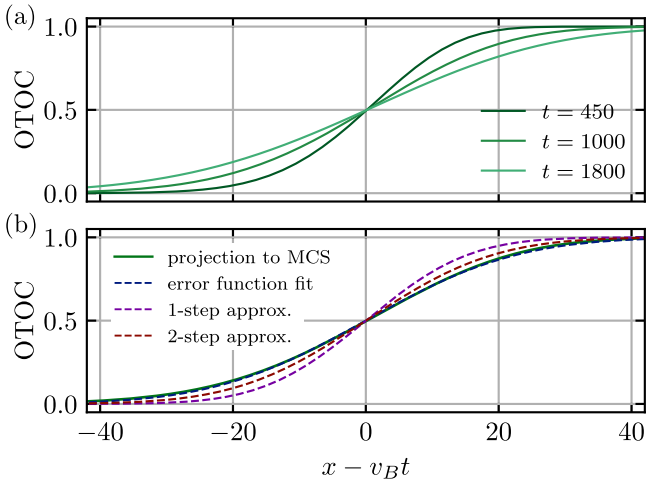

Figure 2: (a) OTOC profile obtained for a representative non-dual-unitary circuit at different times through the developed path-integral formalism. (b) Numerically obtained profile compared with a fit to an error function, and analytically obtained profiles through a controlled expansion of the OTOC in restricted scattering paths.

Conclusion. We developed a numerically tractable discrete path-integral formalism for the out-of-time-order correlator in unitary circuit models of many-body dynamics. This approach predicted a ballistic spreading of the operator front accompanied by a diffusive broadening, hallmarks of generic one-dimensional chaotic quantum many-body dynamics. The butterfly velocity and diffusion constant were shown to be determined by a small set of microscopic quantities set by the operator entanglement of the unitary gates. This approach is well controlled in the limit where the constituting gates are close to the dual-unitary limit, but we argued that it captures the relevant characteristics of scrambling on intermediate to long timescales even for generic circuits. For concreteness, we focused on out-of-time-order correlators, but this approach can be directly generalized to different dynamical probes including Rényi (operator) entanglement, spectral form factors, and deep thermalization. One direct application is in Hayden-Preskill protocols, which probe the capability of information recovery from local subsystems after unitary dynamics [5]. In this way the developed formalism sheds light on universal aspects of the dynamics of quantum information and scrambling.

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2.4 Diagnostics of quantum chaos in multi-unitary kicked Ising dynamics

GIUSEPPE DE TOMASI, MICHAEL A. RAMPP, SUHAIL A. RATHER, AND PIETER W. CLAEYS

Introduction. Understanding the emergence of statistical mechanics from the out-of-equilibrium dynamics of quantum many-body systems is an active research front with many potential applications in quantum technologies. This emergence is deeply connected to the notion of ergodicity in the Hilbert space: Initial wave functions are expected to spread and delocalize in Fock space, approaching a long-time state that is indistinguishable from a purely (Haar) random state. The resulting Haar random states, in turn, present a valuable practical resource for quantum information, quantum tomography, benchmarking of quantum devices, and quantum communication. Indeed, Hilbert space delocalization has very recently gained intense interest in the context of quantum computing, being the backbone of quantum random sampling – the leading test of quantum advantage.

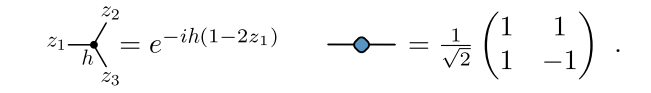
In Ref. [1] diagnostics from quantum computation were applied to many-body quantum dynamics, connecting the universality of quantum computation to notions of quantum chaos and ergodicity. The fundamental object in quantum random sampling is the probability distribution of the Fock-space amplitudes, returning the celebrated *Porter-Thomas distribution* for Haar random states. Focusing on the kicked Ising model at the self-dual point as a minimal model for quantum chaos, the emergence of this Porter-Thomas distribution was established both numerically and analytically. At this maximally chaotic point this convergence was shown to happen exponentially fast in time, with a time scale that is independent of system size. The 'chaoticity' of the quantum many-body dynamics directly translates to the rate with which this distribution emerges, slowing down away from the self-dual point.

The maximal chaos of the self-dual kicked Ising model is underlaid by a duality between space and time. In Ref. [2], different extensions of the self-dual kicked Ising model were proposed that exhibit different symmetries in space-time. These symmetries naturally relate to the presence of kinetic constraints, e.g. in the Floquet east model, and it was shown how these constrain the dynamics of quantum information through the framework of *entanglement membrane theory* (EMT).

Kicked Ising model. We consider the self-dual kicked Ising model, a paradigmatic model of chaotic many-body dynamics. This model describes the dynamics of a one-dimensional chain of spin-1/2 degrees of freedom, where dynamics under a classical Ising Hamiltonian is periodically alternated with a kick along the transverse direction. The Floquet unitary describing a single evolution period of the kicked Ising model is given by $U_F = \exp[-iH_{\mathrm{K}}]\exp[-iH_{\mathrm{I}}]$, generated by the Hamiltonians

$$H_{\mathrm{I}} = J\sum_{j=1}^{L-1}\sigma_j^z\sigma_{j+1}^z + \sum_{j=1}^{L} h_j\sigma_j^z, \quad H_{\mathrm{K}} = b\sum_{j=1}^{L}\sigma_j^y. \quad (1)$$

Here σ_j^α with $\alpha \in \{x, y, z\}$ are the Pauli matrices, L is the length of the chain, J and b are the Ising interaction strength and the transverse kick strength, respectively. $\{h_j\}$ describes a (possibly inhomogeneous) longitudinal field. We fix $J = b = \pi/4$, corresponding to the self-dual point [3,4]. The unitary evolution operator can be graphically represented as in Fig. 1(a) by introducing tensors of the form:



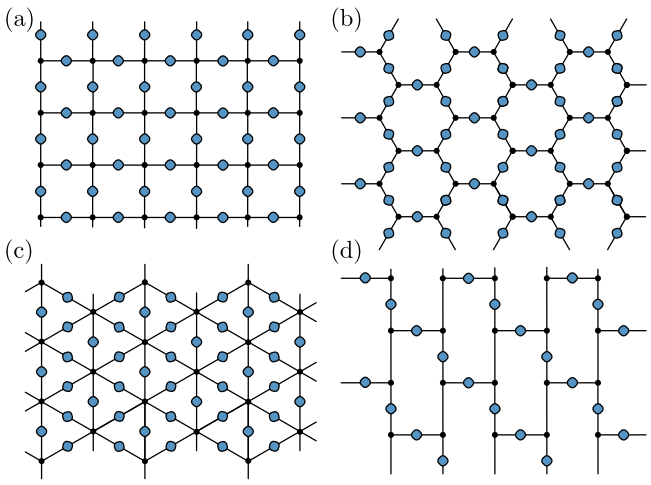


Figure 1: Graphical representation of the unitary evolution operator for different choices of kicked Ising dynamics. Discrete space and time run horizontally and vertically, respectively. The different space-time symmetries correspond to those of (a) the square lattice, (b) the honeycomb lattice, (c) the triangular lattice, and (d) a sheared square latice. All phases have been made implicit.

Emergence of the Porter-Thomas distribution. The resulting dynamics is chaotic and no exact statement can be made about the dynamics of any specific state. Statistical properties can however be analytically determined. Quantum random sampling characterizes the distribution of measurement outcome probabilities $\{p_z = |\langle z|\psi\rangle|^2\}$, where $z = z_1, z_2, \ldots z_L$ with $z_j \in \{0, 1\}$ describing a Fock (bit-string) state. For Haar-random states this distribution returns the Porter-Thomas (or exponential) distribution. In the kicked Ising model self-duality implies that the sampling over measurement outcomes can be interpreted as sampling different measurement-based quantum computations along

the spatial direction. If these perform a universal quantum computation, the emergent randomness corresponds to Haar-randomness in a temporal Hilbert space. After a modest number of discrete time steps, this randomness is indistinguishable from that exhibited by a Haar-random state in the physical Hilbert space (see Fig. 2).

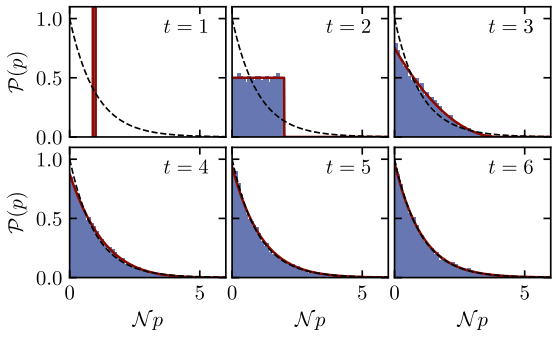


Figure 2: Distribution of bit-string probabilities/overlaps $p = |\langle z|\psi(t)\rangle|^2$ at different times. Numerical results (histograms) are compared with analytical predictions (full red lines), showing excellent agreement. After $t = 6$ discrete time steps, the distribution is visually indistinguishable from the Porter-Thomas distribution (dashed line). Parameters $h_j = \pi/3, \forall j$, system size $L = 14$, and Hilbert space dimension $\mathcal{N} = 2^L$.

Multi-unitary dynamics. Rather than considering the kicked Ising dynamics of Eq. (1), it is possible to devise driving protocols in which Ising phases and quantum kicks are applied alternatingly on different sites. As discussed in Ref. [2], in this way different protocols can be realized for which the unitary evolution exhibits different symmetries in space-time (see Fig. 1). These model do not exhibit the self-duality of the kicked Ising model, but rather *multi-unitarity*. While these models are no longer maximally chaotic, their operator dynamics still allow for an effective description through entanglement membrane theory (EMT). Entanglement membrane theory is an effective coarse-grained description of entanglement growth in chaotic many-body systems, where the fundamental quantity is the entanglement line tension $\mathcal{E}(v)$: For a bipartition of the unitary evolution operator in space-time along a cut $x = vt$, the entanglement scales as $\mathcal{E}(v)t$. While EMT theory in principle applies to generic many-body systems, the need to determine this line tension prevents its application beyond certain fine-tuned or random models. Multi-unitarity however imposes strong constraints on the entanglement line tension, which allow for an exact determination of the entanglement line tension (see Fig. 3), in turn directly returning various quantifiers of operator dynamics including the butterfly and entanglement velocity.

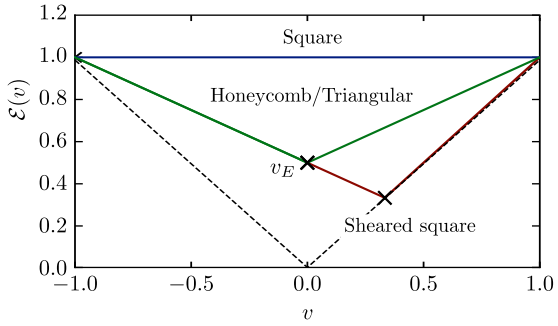


Figure 3: Entanglement line tension $\mathcal{E}(v)$ as a function of the slope v in space-time for dynamics with different space-time symmetries. Multi-unitarity allows the ELT to be fully characterized as a piecewise linear function, with $\mathcal{E}(v = 0)$ corresponding to the entanglement velocity v_E.

Conclusion. We investigated different probes of quantum ergodicity and chaos in multi-unitary kicked Ising models. In the self-dual kicked Ising model it was shown how standard tests of quantum advantage in quantum computation relate to the ergodicity of the corresponding quantum dynamics. This process is governed by delocalization in Hilbert space, which was shown to occurs on a time scale independent of system size – unlike in generic dynamics where it scales logarithmically with system size. This rapid delocalization also highlights how global properties of a quantum state can appear fully ergodic on short time scales even with local properties, e.g. subsystem entanglement, far from their ergodic values. We could gain analytical understanding by interpreting the dynamics as a measurement-based quantum computation in the spatial direction, enabled by the spatial unitarity of the dynamics. By extending the kicked Ising dynamics to different space-time geometries, multi-unitary dynamics can be realized. These dynamics shed light on entanglement membrane theory in microscopic Floquet lattice models, the effective theory through which entanglement dynamics is understood, and enable us to perform nontrivial checks on the validity of its predictions by comparison to exact and numerical calculations.

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2.5 Signatures of the quantum skyrmion Hall effect in the Bernevig-Hughes-Zhang model

ASHLEY M. COOK

Considerable progress has been made to map out the landscape of topologically non-trivial phases of matter since these pioneering efforts [1–3], recently leading to discovery of a generalisation from the framework of the QHE to that of the quantum skyrmion Hall effect (QSkHE) [5, 13]. We characterise this topology in the Bernevig-Hughes-Zhang (BHZ) model. We therefore review a minimal action for the QSkHE in terms of a mixture of two Cartesian spatial coordinates and two extra fuzzy dimensions from separate work [5],

$$S_{CS} = C_2 \int d^3xk\, Tr\left[Tr(G)\, CS_3 \wedge \hat{F}\right], \tag{1}$$

$$CS_3 = \left[AdA + \frac{2}{3}AAA\right], \tag{2}$$

$$\hat{F} = [X_a, A_b] - [X_b, A_a] + [A_a, A_b] - C^c_{ab}A_c, \tag{3}$$

where C_2 is the second Chern number, CS_3 is the standard 2+1 D non-Abelian Chern-Simons Lagrange density, and $\hat{F}$ is the field strength defined over a fuzzy coset space $(SO(5)/SU(2))_F \cong S^2_F$, where S^2_F is the fuzzy two-sphere [1,5,13], expressed in terms of $N \times N$ matrix Lie algebra generators $\{X_a\}$, gauge field components $\{A_a\}$, and structure constant C^c_{ab}. $Tr(G)$ is the trace over the gauge group G, and kTr is the normalised trace over fuzzy coset space coordinates. From this perspective, the minimal phenomenology of the QSkHE relevant to the BHZ model is that of the 4+1 D QHE [8, 26] and 4+1 D CI [17] in higher symmetry cases [5], but with replacement of Landau levels (LLs) by *severely-fuzzified Landau levels*, or LL$_{\text{F}}$s [5].

Hamiltonian—We consider the Bernevig-Hughes-Zhang (BHZ) model [10, 17], with Hamiltonian

$$\mathcal{H} = \sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} H(\boldsymbol{k}) \psi_{\boldsymbol{k}}, \tag{4}$$

in terms of Bloch Hamiltonian $H(\boldsymbol{k})$, with momentum $\boldsymbol{k} = (k_x, k_y)$, and basis vector $\psi^\dagger_{\boldsymbol{k}} = \left(c^\dagger_{\boldsymbol{k},\uparrow,\alpha}, c^\dagger_{\boldsymbol{k},\uparrow,\beta}, c^\dagger_{\boldsymbol{k},\downarrow,\alpha}, c^\dagger_{\boldsymbol{k},\downarrow,\beta}\right)$, where $c^\dagger_{\boldsymbol{k},\sigma,\ell}$ creates a fermion with momentum $\boldsymbol{k}$, spin $\sigma \in \{\uparrow, \downarrow\}$, and orbital angular momentum (OAM) $\ell \in \{\alpha, \beta\}$. In this basis, the Bloch Hamiltonian $H(\boldsymbol{k})$ takes the following form in terms of Kronecker products of Pauli matrices, $\tau^i\sigma^j$

$$\begin{aligned} H(\boldsymbol{k}) = {} & d_z(\boldsymbol{k})\tau^0\sigma^z + d_x(\boldsymbol{k})\tau^z\sigma^x + d_y(\boldsymbol{k})\tau^0\sigma^y \\ & + c_A\tau^x\sigma^y + c_R(f_x(\boldsymbol{k})\,\tau^x\sigma^0 + f_y(\boldsymbol{k})\,\tau^y\sigma^0) + \boldsymbol{h}\cdot\boldsymbol{\tau}\sigma^0. \end{aligned} \tag{5}$$

Here, the $\boldsymbol{d}$-vector $\boldsymbol{d}(\boldsymbol{k}) = (d_x(\boldsymbol{k}), d_y(\boldsymbol{k}), d_z(\boldsymbol{k}))$ is taken to have components as $d_x(\boldsymbol{k}) = \sin(k_x)$, $d_y(\boldsymbol{k}) = \sin(k_y)$, and $d_z(\boldsymbol{k}) = u + \cos(k_x) + \cos(k_y)$, and u is as an effective mass. c_A denotes atomic spin-orbit coupling (SOC) strength and c_R denotes Rashba SOC strength. $\boldsymbol{f}$ is a vector $\boldsymbol{f}(\boldsymbol{k}) = (f_x(\boldsymbol{k}), f_y(\boldsymbol{k}), f_z(\boldsymbol{k}))$ with components $f_x(\boldsymbol{k}) = \sin(k_y)$, $f_y(\boldsymbol{k}) = -\sin(k_x)$ and $f_z(\boldsymbol{k}) = 0$. $\boldsymbol{h} = (h_x, h_y, h_z)$ encodes an effective Zeeman field, where $\boldsymbol{\tau} = (\tau^x, \tau^y, \tau^z)$ is a vector of Pauli matrices.

Orbital angular momentum textures in momentum-space and real-space for finite Zeeman field—To characterise signatures of the quantum skyrmion Hall effect (QSkHE) in the BHZ model, we introduce the skyrmion number [15] as

$$\mathcal{Q} = \frac{1}{4\pi}\int_{BZ} d\boldsymbol{k} \langle \boldsymbol{S}(\boldsymbol{k})\rangle \cdot \left(\partial_{k_x}\langle \boldsymbol{S}(\boldsymbol{k})\rangle \times \partial_{k_y}\langle \boldsymbol{S}(\boldsymbol{k})\rangle\right), \tag{6}$$

where $\langle \boldsymbol{S}(\boldsymbol{k})\rangle = (\langle S_x(\boldsymbol{k})\rangle, \langle S_y(\boldsymbol{k})\rangle, \langle S_z(\boldsymbol{k})\rangle)$ is the ground-state OAM expectation value computed as $\langle S_i(\boldsymbol{k})\rangle = \sum_n^{occ}\langle n, \boldsymbol{k}|S_i|n, \boldsymbol{k}\rangle$, where $|n, \boldsymbol{k}\rangle$ is the Bloch eigenstate for the n^{th} lowest-energy band at momentum $\boldsymbol{k}$, and n runs over occupied states. Here, we assume half-filling of the bands. Unless stated otherwise, the matrix representations of the OAM operators are taken to be $S_x = \tau^z\sigma^x$, $S_y = \tau^0\sigma^y$, and $S_z = \tau^0\sigma^z$.

Bulk-boundary correspondence under weak Zeeman field—We now characterise bulk-boundary correspondence of the BHZ model consistent with the QSkHE. Bulk-boundary correspondence under TRS is shown in Fig. 1 a) for open-boundary conditions (OBCs) in the $\hat{x}$-direction. Helical edge states are observed, which appear to be those of the QSHI. They evolve to unexpected edge states at finite Zeeman field strength, however, as shown in Fig. 1 b). The slab spectrum is gapless as expected at two finite k_y values, but an unexpected finite hybridisation gap Δ, is observed at $k_y = 0$, such that individual bands in the gap *delocalise* at $k_y = 0$. Within the QSkHE, this hybridisation gap Δ is a signature of an intrinsically 4+1 D topological phase, due to two Cartesian spatial coordinates, and two spatial dimensions encoded in the OAM operator matrix representations and Lie algebra [5]. $\mathcal{Q}$ characterises this higher-dimensional topology, being similar to a second Chern number [5], and the gapless points in the slab spectrum correspond to WN$_{\text{F}}$s.

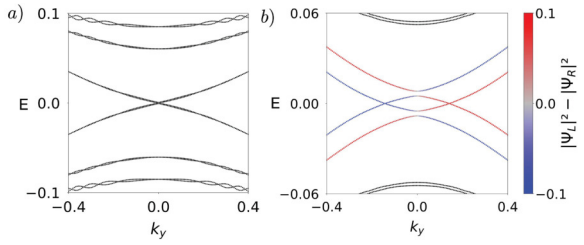

Figure 1: a) Slab spectrum for OBCs in the $\hat{x}$-direction with parameter set $u = -1.56$, $c_A = -0.77$, and $\boldsymbol{h} = 0$. b) slab spectrum as in a) except $\boldsymbol{h} = 0.14\hat{z}$. Color bar characterises localisation of in-gap states. System size in the $\hat{x}$-direction is $N = 100$.

Unexpected edge conduction from compactified 3D Weyl nodes WN$_F$s—In this section, we first briefly review past joint theoretical-experimental work on HgTe quantum wells (QWs) [12]. In this past work, unexpected conduction at two edges is reported for HgTe QWs realising the QSHI phase, in the presence of a finite Zeeman field and orbital magnetic field, which was not explained. Given discovery of the QSkHE and these past unexplained experiments, we investigate effects of interplay between Zeeman and orbital magnetic fields on the WN$_F$s. Modeling magnetic disorder in terms of random in-plane Zeeman field components, we find the spectrum for OBCs in each of the $\hat{x}$- and $\hat{y}$-directions remains gapless for finite disorder strength, as shown in Fig. 2 a), consistent with interpretation of zero-energy gapless points in Fig. 1 b) as WN$_F$s, given robustness of 3D Weyl nodes [17]. Computing the slab spectrum for OBCs in the $\hat{x}$-direction without disorder but with weak rotation of the applied Zeeman field away from the $\hat{z}$-axis, we find the slab spectrum develops a finite minimum direct gap, but also a negative indirect gap for these OBCs, as shown in Fig. 2 b).

We distinguish between orbital field strengths B less than and greater than a critical value B_c, which corresponds to a bulk gap-closing marked by dashed blue lines, shown in Fig. 2 c). LDOS for $B < B_c$ is shown in Fig. 2 d) (top) and LDOS for $B > B_c$ is shown in Fig. 2 d) (bottom), indicating edge conduction persists to field strengths beyond B_c.

In summary, we characterise the BHZ model from the perspective of the quantum skyrmion Hall effect (QSkHE) framework in this work [5, 13]. We identify signatures of topological skyrmion phases of matter [15], which are compactified 4D Chern insulators within the QSkHE, exhibiting compactified 3D Weyl nodes (WN$_F$s) at the boundary. Response of WN$_F$s to application of weak Zeeman and orbital magnetic fields is consistent with past experimental observation of unexpected edge conduction in HgTe quantum wells [12]. This experimental work by Ma *et al.* [12] therefore potentially constitutes the first known experimental observation of signatures of the QSkHE beyond the simpler framework of the quantum Hall effect.

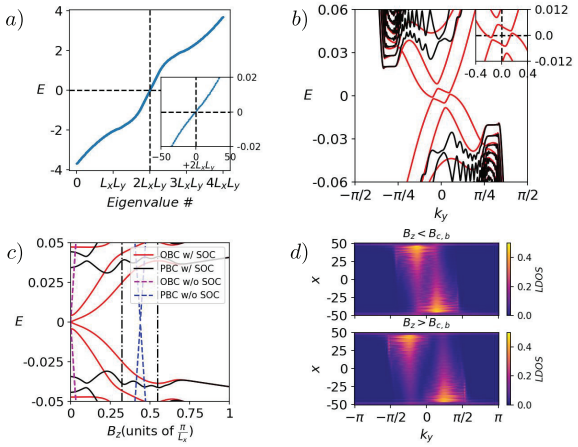

Figure 2: For parameters $u = -1.56$, and $c_A = -0.77$, a) energy eigenvalues vs. eigenvalue index for OBCs in each direction with $L_x = L_y = 101$, and $h_z = 0.12B_z$ with $B_z = 0.003$ in presence of disorder in $\boldsymbol{h}_{\parallel} = (h_x, h_y)$ in the range $(-0.05, 0.05)$ averaged over 50 disorder realisations with inset showing spectrum close to zero energy, b) slab spectra vs. k_y with both PBCs (black) and OBCs (red) for $L_x = 101$ and tilted Zeeman field with $\boldsymbol{h} = 0.03\hat{x} + 0.04\hat{y} + 0.12B_z\hat{z}$ and $B_z = 0.003$ with inset showing dispersion close to zero energy, c) energy vs. orbital out-of-plane magnetic field, B_z, at $k_y = 0$ with PBCs (black) and OBCs in the $\hat{x}$-direction(red) and same for $c_A = 0$ with PBCs (blue) and OBCs(magenta), d) LDOS for energy $E = 0$ vs. k_y and x for $B_z = 0.010$ (top) and $B_z = 0.017$ (bottom) denoted by dash-dotted black vertical lines in c).

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2.6 Effective field theory of the quantum skyrmion Hall effect

ASHLEY M. COOK

At the frontiers of modern physics, interpretation and treatment of spin angular momentum in quantum mechanics is still being expanded to confront the challenges of unification of the four forces. Spin angular momenta associated with matrix Lie algebras have emerged as useful tools in encoding spatial dimensions [1–10]. While spin angular momentum is used in these effective theories to encode spatial dimensions to great effect when the matrix representation size of the Lie algebra generators is large (generators are represented by $N \times N$ matrices, with N large) [11, 12], spin angular momentum is treated as a quantum number—effectively as just a label—for quantum states when N is small, such as in study of quantum spin liquids and other strongly-correlated phases of matter. In this small N regime, spin is termed isospin specifically to convey it is an internal degree of freedom (DOF). It is also termed (pseudo)spin (pspin) in the condensed matter literature, to convey that it could be associated with the physical spin or some other DOF, such as a layer or valley DOF.

One can then ask, are these two treatments of spin angular momentum in quantum systems—at large N and at small N—consistent? If so, how exactly does the cross-over from interpretation of spin as encoding spatial dimensions at large N to interpretation of spin as a label at small N occur? This question is deeply relevant to the quantum skyrmion Hall effect (QSkHE) [13] and related topologically non-trivial phases of matter [14–16] recently-identified in condensed matter systems, and we address it as part of introducing the effective field theory (EFT) of the QSkHE. We find that spin angular momentum encoded in matrix Lie algebras may encode intrinsically $\delta + 1$ (δ spatial dimensions and 1 time dimension) dimensional topologically non-trivial phases of matter, even for small non-trivial N in the regime where spin has previously been treated as a label [17]. A system with D Cartesian space coordinates and δ dimensions encoded in spin angular momentum can then potentially realise states of intrinsic dimensionality $D + \delta + 1$.

Based on this generalisation to interpretation of spin as encoding some number of spatial dimensions, even for small matrix representation size of the associated matrix Lie algebra generators, we introduce an EFT for the QSkHE consistent with a growing number of related works [14–16, 18–25], by generalising quantum field theories with extra fuzzy dimensions [1, 2, 4], defined over manifolds with global product structure, to those with local product structure, and retaining dependence on fuzzy gauge fields in the small N regime.

Gauge theory over fuzzy spaces—Following Aschieri *et al.* [4], we decompose the field strength F_{MN} in terms of a component defined over the remaining Cartesian coordinates as $F_{\mu\nu}$, a component defined over the fuzzy sphere as F_{ab}, and a mixed term $F_{\mu a}$, which take the following forms:

$$\begin{aligned} F_{\mu\nu} &= \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]\,, \\ F_{ab} &= [X_a, A_b] - [X_b, A_a] + [A_a, A_b] - C^c_{ab} A_c \\ F_{\mu a} &= \partial_\mu A_a - [X_a, A_\mu] + [A_\mu, A_a] \end{aligned} \tag{1}$$

For the present purposes, we apply this machinery to a simplification of the 4+1 D SU(2) gauge theory for the QHE. We consider the flat space limit of this theory [26], in which the theory decomposes into a theory of two 2+1 D QHEs, such as over the xy plane and the zw plane. We may then write the gauge theory of the 4+1 D QHE as an Abelian $U(1)$ CS action over $M^{1,2} \times S^2$,

$$S_{CS} = C_2 \int d^5x \; AdAdA, \tag{2}$$

where here the second Chern number C_2 is a product of two first Chern numbers, one for each 2+1 D QHE, or C_{xy} and C_{zw}, respectively. That is, $C_2 = C_{xy} C_{zw}$.

This theory possesses a product structure amenable to fuzzifying two spatial dimensions within the framework of extra fuzzy dimensions. We fuzzify S^2, yielding the action for the theory in terms of a mixture of two Cartesian spatial coordinates and two extra fuzzy dimensions as,

$$S_{CS} = C_2 \int d^3x k \; Tr\left[Tr(G)\; CS_3 \wedge \hat{F}\right] \tag{3}$$

$$CS_3 = \left[AdA + \frac{2}{3} AAA\right] \tag{4}$$

$$\hat{F} = [X_a, A_b] - [X_b, A_a] + [A_a, A_b] - C^c_{ab} A_c, \tag{5}$$

yielding an action similar in form to a strictly 2+1 D CS action save for a particular matrix structure.

Computing topological invariants on severely-fuzzified spaces or for extra severely-fuzzified dimensions—We propose topological invariants for fuzzy coset spaces corresponding to finite matrix dimension N, by considering field strength components $F_{ab,s}$ as

$$F_{ab,s} = \left[S_a, A^b\right] - [S_b, A^a] + \left[A^a, A^b\right] - C^c_{ab,occ} A^c. \tag{6}$$

The expected expression for topological charge q of a $\mathrm{LL_F}$ more generally is then,

$$\begin{aligned} q &= k \,\mathrm{tr}\,[\boldsymbol{C}] \\ &= k \,\mathrm{tr}\left[[F_{ab,s}, F_{bc,s}]\, F^{-1}_{ca,s}\right], \end{aligned} \tag{7}$$

which is the fuzzified counterpart of the topological charge q of a skyrmion in a NLσM appearing as central extension of a momentum commutator [28]. It is useful to note that this algebra generally corresponds to some topological deformation of a fuzzy two-sphere, which we term the fuzzy topological two-sphere ($S^F_{(T)F}$).

This work introduces the effective field theory (EFT) of the quantum skyrmion Hall effect (QSkHE), a generalisation of the quantum Hall effect (QHE) framework, in which intrinsically $\delta+1$-dimensional (δ+1 D, $\delta > 0$) compactified many-body states defined over severely-fuzzified manifolds can play the role in QSkHE that charged particles play in QHE. This is consistent with the interpretation that (pseudo)spin (pspin) degrees of freedom (DOFs), where pseudo indicates the spin could correspond to myriad physical quantities, associated with matrix representation size of associated Lie algebra generators $N \times N$, encode δ spatial dimensions both with large N, as considered before in study of non-commutative field theories [1–4, 11], but also when N is small and the pspin DOF is interpreted as isospin, or internal DOF. This EFT is developed to explain phenomenology of the QSkHE identified in other works [13–16], which indicate topological states of myriad isospin DOFs in systems with d Cartesian space coordinates show bulk-boundary correspondence and response signatures identifiable with known d +δ+1 D topologically non-trivial phases of matter.

In summary, this work centers on the interpretation of spin angular momentum encoded in a matrix Lie algebra with generators of matrix representation size $N \times N$, where N is potentially small. This is the regime where spin has previously been treated as a label, rather than as encoding spatial dimensions as in more recent works on non-commutative field theories [1–4,11]. The QSkHE and its EFT reveal spin angular momentum encodes some finite number of spatial dimensions even for small N, in general, contrary to past theoretical treatments, in the sense that spin angular momentum can encode an intrinsically δ+1 D topologically non-trivial many-body state in this regime of small N. Such many-body states can furthermore play the role in the QSkHE that charged particles play in the QHE, yielding intrinsically d+δ+1 D states in systems with d Cartesian space coordinates as well as pspin DOFs encoding δ dimensions in fuzzy coset space coordinates. This motivates review of myriad problems of quantum mechanics involving spin angular momentum encoded in matrix Lie algebras, and reveals the significant impact discovery the QSkHE and this interpretation of spin could have on quantum information and related problems in many areas of modern physics.

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2.7 Quantum many-body control using reinforcement learning with tensor networks

FRIEDERIKE METZ AND MARIN BUKOV

Introduction and Motivation Critical states exhibit non-trivial correlations and strong system-size dependence, making their manipulation challenging. Adiabatic preparation of critical states becomes increasingly time-prohibitive as particle number grows, while sweeping through critical points reveals universal properties. Developing optimal control strategies beyond the adiabatic limit is thus crucial. Critical state preparation is also vital for quantum metrology, where the heightened sensitivity of critical states to external fields enables more precise measurements.

Inspired by Ref. [1] we introduce a deep reinforcement learning (RL) framework for quantum many-body control using matrix product states (MPS) [Fig. 1]. MPS are employed both to describe quantum states and represent the RL agent, leading to a hybrid MPS-neural network (QMPS) that scales linearly with system size. This approach enables the control of larger quantum systems, unlike full wavefunction methods.

As a case study, we focus on state preparation for the mixed-field Ising chain. QMPS agents generate control protocols that can generalize to unseen states and adapt to noise [2]. Unlike traditional quantum control methods (e.g., CRAB, GRAPE), RL agents retain their control policy after training, making them robust and efficient even under stochastic dynamics.

Our MPS-based RL framework is tailored for preparing low-entangled states in 1D, such as ground states of local gapped Hamiltonians. We focus on the 1D mixed-field Ising model, described by:

$$\hat{H}_{\text{Ising}} = J \sum_{j=1}^{N-1} \hat{Z}_j \hat{Z}_{j+1} - g_x \sum_{j=1}^{N} \hat{X}_j - g_z \sum_{j=1}^{N} \hat{Z}_j, \quad (1)$$

where g_x (g_z) denotes the transverse (longitudinal) field. The system on lattice site j is described using the Pauli matrices X_j, Y_j, Z_j. For $g_z > 0$, the model has no known closed-form expressions for its eigenstates and eigenenergies. The phase diagram features a critical line from $(g_x, g_z) = (1, 0)$ to $(g_x, g_z) = (0, 2)$ marking a transition from a paramagnetic to an antiferromagnetic phase.

We now show how the RL agent prepares a ground state in the critical region of the mixed-field Ising chain ($J = +1, g_x = 0.5, g_z = 1.5$) starting from non-critical paramagnetic ground states of the same model but with flipped interaction strength $J = -1$, $1.0 < g_x < 1.5$, $0 < g_z < 0.5$. Thus, the agent learns to connect ground states of two distinct Hamiltonians.

We train our QMPS agent on $N = 16$ spins with a single-particle fidelity threshold of $F^*_{\text{sp}} = 0.97$ ($F^* \sim 0.61$) and a maximum episode length of 50. Figure 2(a) shows the fidelity between the target and final states for various initial ground states in a rectangular region of the (g_x, g_z)-plane. The agent generalizes well to unseen initial states far outside the training region (white rectangle), failing only near the critical point of the transverse field Ising model ($g_x = 1, g_z = 0$) and for a few isolated initial states well beyond the training region.

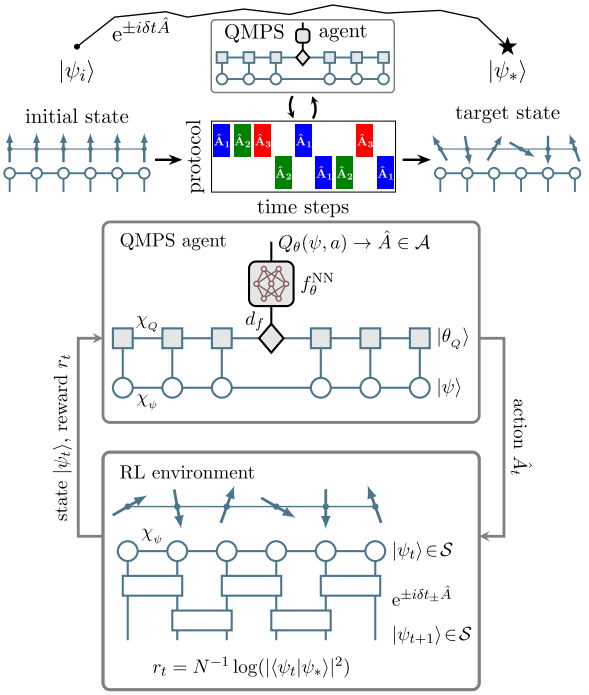

Figure 1: We transfer population from an initial to a target ground state of the mixed-field Ising model using an RL agent to construct a step-by-step gate protocol. The optimized agent outputs a sequence of operators $\hat{A}_j$ that evolve the initial spin state into the target state (marked by a star). The RL agent leverages a deep-learning architecture (QMPS) based on a matrix product state and is trained using the deep Q-learning algorithm [2].

Results We demonstrate the QMPS agent's remarkable generalization capabilities in noisy environments, analyzing its robustness to stochastic perturbations in state evolution—a common challenge in noisy intermediate-scale quantum (NISQ) devices. Two independent noise sources are considered: (i) At each time step, with probability ϵ, a random action replaces the selected one, simulating bit- or phase-flip errors common in quantum computing. (ii) Gaussian noise with zero mean and standard deviation σ is added to the time duration $\delta t_\pm$ of each unitary operator, mimicking imperfect experimental controls.

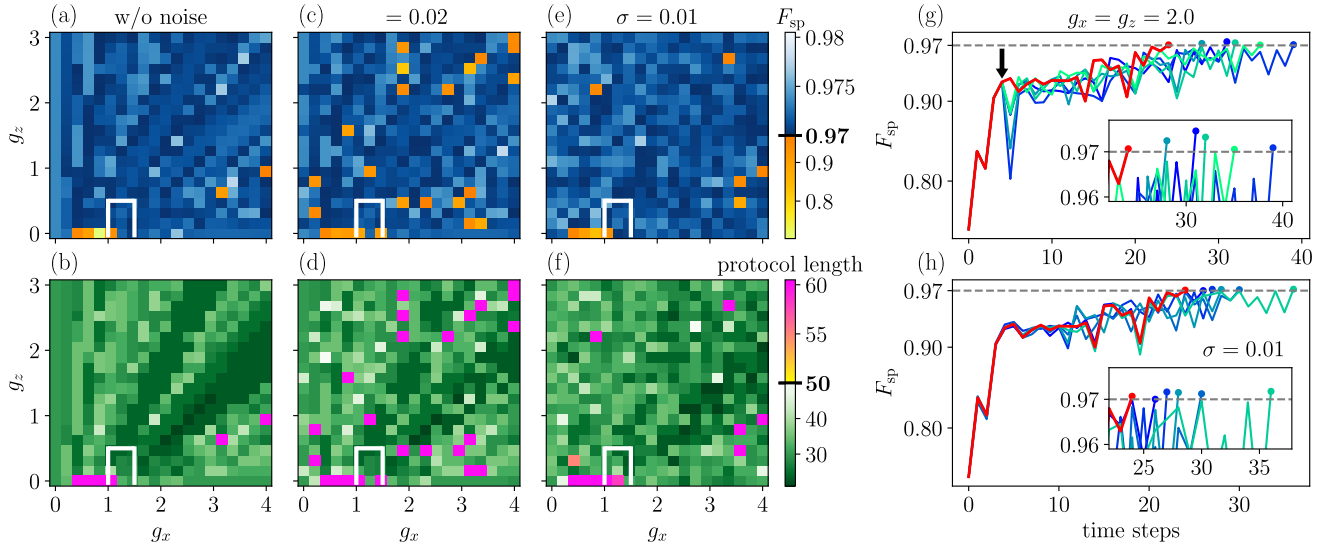

Figure 2: (a),(b) Final single-particle fidelity $F_{\rm sp} = \sqrt[N]{F}$ [top] and corresponding protocol length [bottom] – see colorbars – versus the initial Ising ground state parameter values g_x, g_z. The target is a state in the critical region of the Ising model at ($J=+1, g_x=0.5, g_z=1.5$). Trained only on initial states sampled randomly from the enclosed white rectangle. Each of the two parts of a colorbar is shown on a linear scale with the fidelity threshold ($F^*_{\rm sp}=0.97$, $F^*\sim 0.61$) and the maximum episode length during training (50), indicated by short black lines. (c)-(f) Same as (a)-(b) but for noisy evolution – (c),(d): At each time step, actions other than the one selected by the agent, are taken with probability $\epsilon = 0.02$; (e),(f): Whereas Gaussian noise with standard deviation $\sigma = 0.01$ is added to the time step $\delta t_\pm$ of all applied unitaries. (g) Time evolution of single-particle fidelity starting from an arbitrary initial ground state, following the protocol constructed by the trained agent. The red curve shows the noise-free QMPS protocol. At time step 5 (black arrow), the protocol is perturbed by enforcing five suboptimal actions. All subsequent actions are selected according to the trained QMPS policy without further perturbation (blue curves). The inset highlights fidelity near the threshold (dashed gray line), showing all protocols successfully terminated. (h) Same as (g), but with Gaussian noise applied at every $\delta t_\pm$. $N=16$ spins.

Noise type (i) is equivalent to using an ϵ-greedy policy. Hence, the states encountered could have been visited during training. Due to the generalization capabilities of RL, the agent acts optimally after non-optimal actions have occurred, attempting to correct for the 'mistake'. Fig. 2(c-d) shows the achieved final fidelity [top] and the required number of steps [bottom] for $\epsilon=0.02$; the fidelity threshold can be reached in the majority of test cases. The randomness results in longer protocols indicating that the agent adapts to encountered states. In the noise-free case, the agent fails to prepare the target state for a few points outside the training region [orange points in Fig. 2(a)] due to not fully converged Q-values outside the training region. After adding the perturbation, the agent is able to correct its mistake [Fig. 2(c)].

We use distinct time steps, $\delta t_\pm$, for positive and negative actions, allowing the agent to adjust the entire sequence of unitaries in a non-trivial manner rather than undoing a non-optimal action with its inverse. The QMPS agent's adaptability is shown in Fig. 2(g), where the fidelity is plotted during time evolution starting from an arbitrary initial ground state. At $t=5$, the protocol is perturbed by 6 different actions, leading to 6 distinct branches. For each branch, the agent meets the fidelity threshold after a few additional steps.

In contrast to the ϵ-noise, adding Gaussian noise σ, (ii), to the time step duration $\delta t_\pm$, results in states the agent has not encountered during training. This noise tests the agent's ability to generalize beyond training, and interpolate between quantum many-body states. Fig. 2(e)-(f) displays the achieved fidelity and the corresponding protocol length for $\sigma = 0.01$. The QMPS agent remains robust. Fig. 2(h) displays the fidelity trajectories starting from the same initial state using 5 different random seeds, demonstrating that the agent successfully adapts to unencountered many-body states and drives the protocol to meet the fidelity threshold.

The robustness of QMPS agents to noise and stochasticity highlights a key advantage of deep RL over traditional quantum control methods. Conventional techniques perform suboptimally in noisy systems because they do not incorporate quantum state information during time evolution and optimize protocols for specific, fixed quantum state trajectories. In contrast, QMPS value functions are optimized across a range of states, enabling the agent to interpolate and extrapolate to both seen and unseen states, as long as the deep-learning approximation remains accurate. Unlike traditional quantum control algorithms, QMPS agents can automatically self-correct their protocols in real time [2].

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2.8 Making Trotterization adaptive and energy-self-correcting for NISQ devices

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Introduction Quantum computers hold the promise to outperform their classical counterparts in certain tasks, with digital quantum simulation (DQS) of many-body systems attracting considerable attention. DQS of continuous time evolution requires time discretization, e.g., via a Trotterization procedure. A finer time step improves simulation precision, but inevitably leads to increased computational efforts. This is particularly costly for noisy intermediate scale quantum (NISQ) computers, where notable gate imperfections limit circuit depth that can be executed at a given accuracy.

In Ref. [1], we propose the ADA-Trotter algorithm to reduce the cost by exploiting the properties of the evolved state: at a fixed evolution time, a larger δt can give rise to a shorter gate sequence in time windows when the state changes slowly, without incurring a higher error. An essential element of our algorithm is a feedback loop which self-corrects the simulation errors in the conservation of the target Hamiltonian H, through adapting time steps, as summarized in Fig. 1.

More precisely, for a target unitary $U=\exp(-i\delta t H)$ with $H=H_+ + H_-$, we consider an approximate Trotterized unitary operator $U_T(\delta t)=e^{-i\delta t H_-/2}e^{-i\delta t H_+}e^{-i\delta t H_-/2}$. For a given quantum state $|\psi(t_m)\rangle$, we aim to find the largest possible time step δt_m, such that, in the time-evolved state $|\psi(t_m+\delta t_m)\rangle=U_T(\delta t_m)|\psi(t_m)\rangle$, the energy density $\mathcal{E}_{m+1}=L^{-1}\langle\psi(t_m+\delta t_m)|H|\psi(t_m+\delta t_m)\rangle$ and its fluctuations density $\delta\mathcal{E}^2_{m+1}=L^{-1}\langle\psi(t_m+\delta t_m)|H^2|\psi(t_m+\delta t_m)\rangle - L\mathcal{E}^2_{m+1}$, with L the system size, remain both bounded:

$$|\mathcal{E}_{m+1}-\mathcal{E}|<d_{\mathcal{E}}, \qquad |\delta\mathcal{E}^2_{m+1}-\delta\mathcal{E}^2|<d_{\delta\mathcal{E}^2}, \quad (1)$$

where $\mathcal{E}, \delta\mathcal{E}^2$ are the energy and the variance density of the initial state.

These conditions ensure the conservation of average density and its fluctuations, up to the maximally allowed errors $d_{\mathcal{E}}$ and $d_{\delta\mathcal{E}^2}$. Crucially, as we always compare conserved quantities with their initial values, these errors will not accumulate in time. Remarkably, although we only constrain deviations in the lowest two moments of H explicitly, our numerical results suggest that it is sufficient to constrain the higher moments of H. Hence, the target Hamiltonian H emerges as an approximate constant of motion, despite Trotterization explicitly violating its conservation.

Results We illustrate the ADA-Trotter algorithm in a classical simulation and consider a non-integrable quantum Ising model, $H=H_+ + H_-$, as our target Hamiltonian:

$$H_- = J_z\sum_j \sigma^z_j\sigma^z_{j+1} + h_z\sum_j \sigma^z_j, \quad H_+ = h_x\sum_j \sigma^x_j, \quad (2)$$

for a chain of L lattice sites. We consider a uniform nearest-neighbor Ising coupling J_z, and transverse and longitudinal fields h_x and h_z, respectively.

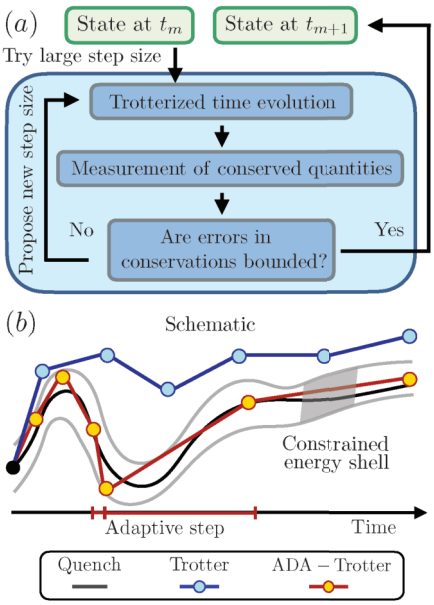

Figure 1: (a) Schematic of the ADA-Trotter protocol. Given a quantum state at time t_m and a Trotter expansion which approximates a target Hamiltonian, one tries to use the largest possible Trotter step size as long as errors in conservation laws are bounded. (b) ADA-Trotter generally outperforms conventional Trotter: States propagated via ADA-Trotter (orange) are constrained in a energy shell where energy and its variance are approximately conserved. In contrast, a fixed step size is chosen for conventional Trotter (blue) and larger errors may occur.

We restrict the simulation to a maximum number of $N=15$ Trotter steps; this is equivalent to limiting the circuit depth, and reflects constraints on present-day NISQ devices. Consider the initial state $\exp(-i\pi\sum_j \sigma^y_j/8)|\downarrow\ \ldots\ \downarrow\rangle$. The dynamics of the magnetization in the x and z directions are shown in Fig. 2 (a) and (b), respectively. At early times, the exact dynamics (black) exhibits rapid oscillations in both observables, which damp out with time. For ADA-Trotter with tight constraints in energy and variance, $d_{\mathcal{E}}=0.03, d_{\delta\mathcal{E}^2}=1$ (orange circles), the exact dynamics is reproduced with high accuracy. We include here both cases of a constrained energy variance with $d_{\delta\mathcal{E}^2}=1$, and of an unconstrained variance $d_{\delta\mathcal{E}^2}=\infty$ (dashed red), to demonstrate the importance of preserving the second moment of energy.

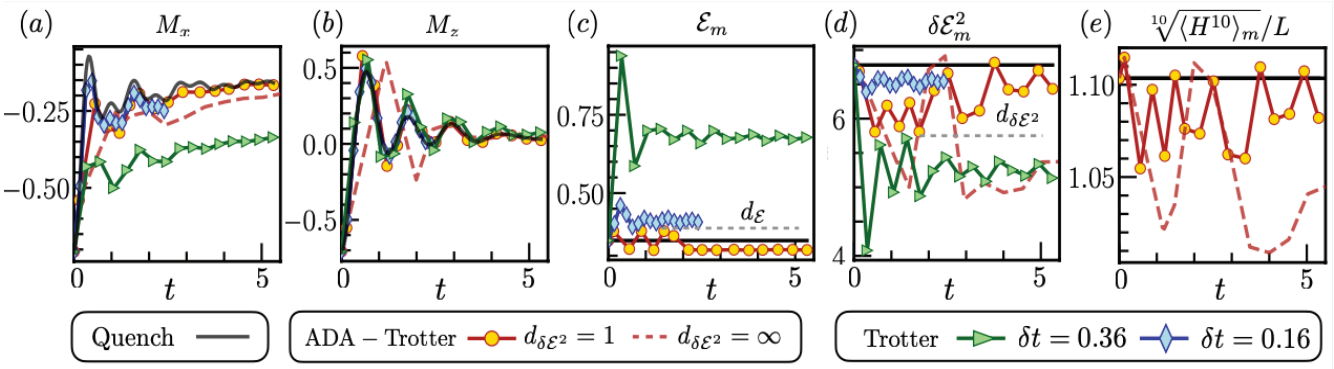

Figure 2: Comparison between ADA-Trotter and fixed step Trotterization. (a) and (b) depict the time evolution of magnetization in x and z direction, respectively. Variance constraint is crucial for ADA-Trotter: with variance constraint $d_{\delta\mathcal{E}^2}=1$ (orange circle) ADA-Trotter reproduces the exact dynamics whereas notable deviation appears for $d_{\delta\mathcal{E}^2}=\infty$ (dashed red) without variance control. ADA-Trotter outperforms fixed step Trotter: For a large fixed trotter step (δt=0.36, green triangle), notable local errors appear at early times; A smaller δt can be employed (blue diamond) to suppress errors but the total simulation time is limited. (c) and (d) depict the expectation value of target Hamiltonian H and its variance, deviations of which are constrained by $d_\mathcal{E}$ and $d_{\delta\mathcal{E}^2}$ for ADA-Trotter. Fixed step Trotter can lead to a sufficiently large error in energy at early times. (e) Higher moments of the target Hamiltonian is better preserved with variance constraint. We use $J_z=-1, h_x=-1.7, h_z=0.5, d_\mathcal{E}=0.03, L=24$ for numerical simulation.

ADA-Trotter can outperform Trotterization with a fixed step size: To reach the same maximal physical simulation time (t≈5.5), we apply Trotterization with a fixed step size δt=0.36 (green triangles), for which notable deviations in M_x appear already at very early times (t≈1); a smaller step size δt=0.16 (blue diamonds) can be chosen to suppress local errors such that they are comparable to ADA-Trotter. However, this comes at a cost of a reduced total simulated time (t≈2.5) which drops by a factor of two compared to ADA-Trotter.

The reason behind the efficiency of ADA-Trotter with tight constraints lies in the self-correction of errors in the conservation law of the target Hamiltonian, a feature that is crucial for a faithful digital simulation but absent in the conventional Trotter scheme. As illustrated in Fig. 2 (c), rather than being a conserved quantity (black), energy density $\mathcal{E}_m$ now becomes time-dependent for ADA-Trotter (orange dots). Remarkably, it fluctuates around the correct value within a controlled error $d_\mathcal{E}$ (grey), signifying that our algorithm is self-correcting the energy errors by adapting the time steps. In contrast, conventional Trotter (green) leads to notable deviations in energy, which saturate quickly at a value far from the black line and cannot be corrected.

Similarly, the energy variance also changes in time and notable deviation from the initial value (black line) can occur if there is no constraint in variance ($d_{\delta\mathcal{E}^2}=\infty$, dashed red line in Fig. 2 (d)). Such a deviation can be controlled by setting $d_{\delta\mathcal{E}^2}=1$ (orange circles). In Fig. 2 (e) we show a higher moment of the target Hamiltonian $\sqrt[n]{\langle H^n\rangle_m}/L$ for $n=10$: remarkably, the errors in this quantity are also constrained at $d_{\delta\mathcal{E}^2}=1$, and grow with $d_{\delta\mathcal{E}^2}$. Hence, enforcing only energy conservation is insufficient, while constraining in addition its variance is necessary to preserve the conservation of the target Hamiltonian. This happens possibly because by central-limit theorem the correct characterization of the energy distribution requires only the first two moments.

ADA-Trotter can be generalized to protect other symmetries in addition to the energy constraints, and to deal with time-dependent Hamiltonians where piecewise "conserved" quantities are used to estimate errors [2]. Although the feedback loop introduces some overhead, it offers a practical way to achieve more accurate simulations on NISQ devices. This approach holds potential for simulating complex quantum dynamics more efficiently than conventional Trotterization methods. In fact, it can be potentially useful on a more general level whenever time discretization is involved; this includes for instance, also numerical approaches based on time-evolving block decimation methods.

[1] H. Zhao, M. Bukov, M. Heyl, and R. Moessner, PRX Quantum **4**, 030319 (2023).

[2] H. Zhao, M. Bukov, M. Heyl, and R. Moessner, Phys. Rev. Lett. **133**, 010603 (2024).

2.9 Finite-Temperature Phenomena in the Doped Hubbard Model: From Forestalled Phase Separation to the Pseudogap

ARITRA SINHA AND ALEXANDER WIETEK

Introduction Experimental studies over the last few decades have identified stripe order as a central feature in the phase diagram of high-temperature cuprate superconductors. The Fermi Hubbard Model (FHM), which captures the essential physics of strongly correlated cuprate systems, is given by the Hamiltonian:

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}\right) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

where t is the nearest-neighbor (NN) hopping amplitude, $U > 0$ is the on-site Coulomb repulsion, $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) create (annihilate) electrons with spin σ at site i, and $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the number operator. The notation $\langle i,j\rangle$ runs over NN sites on the square lattice. Throughout this report, we set $t = 1$ for simplicity. Recent numerical studies have shown that stripe (intertwined charge and spin) order emerges as the ground state of the two-dimensional FHM in certain doping regimes near half-filling and large U. At higher temperatures, well above the stripe-ordered ground state, the system enters the pseudogap and strange-metal regimes, whose microscopic mechanisms remain elusive. Using advanced tensor-network methods—infinite projected entangled pair states (iPEPS) and minimally entangled typical thermal states (METTS)—we show, that at temperatures near the pseudogap regime, doped holes in the Hubbard model can form statistically fluctuating charge clusters reminiscent of phase separation, wherein the system appears to partition into hole-rich and hole-depleted regions [1].

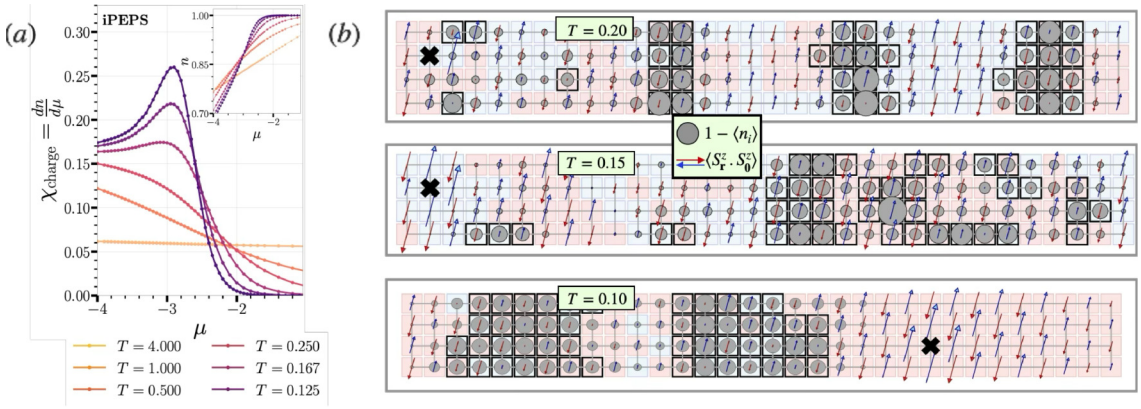

Figure 1: (a) Charge susceptibility χ_{charge} vs chemical potential μ obtained via iPEPS simulations on an infinite square lattice at $U = 10$ for temperatures $T = 4$ down to $T = 0.125$. (b) Hole density and spin correlations for a typical METTS state at $U = 10$ and doping $\delta = 0.0625$ on a 32×4 cylinder. Gray circles at each site l represent the local hole density $1 - \langle n_l \rangle$. Spin correlations are shown by red (negative) and blue (positive) arrows, proportional to $\langle S^z_0 S^z_l \rangle$, with the black cross indicating the origin of the spin correlator. Red and blue squares highlight staggered spin correlations.

Thermodynamic-limit charge susceptibility and lattice snapshots. We perform iPEPS simulations in the two-dimensional thermodynamic limit using a grand canonical ensemble, where we control the filling n by varying the chemical potential μ. Our calculations for charge susceptibility $\chi_{\text{charge}} = \frac{\partial n}{\partial \mu}$ versus doping reveal a maximum around doping $p \approx 1/8$. Figure 1(a) shows, as temperature is lowered, this maximum becomes increasingly sharp, indicating a near-critical instability. A genuine phase-separated state would imply a divergence in χ_{charge}. Instead, our data show a finite peak, pointing to partial or 'incipient' segregation of carriers.

To visualize real-space structure, we use METTS on cylindrical geometries. METTS is a Markov-chain Monte Carlo approach (see Ref. [2] for details) that samples product states $|\sigma_i\rangle$ with probability $p_i = \langle\sigma_i| e^{-\beta H} |\sigma_i\rangle$, then evolves each state in imaginary time to form

$$|\psi_i\rangle = \frac{e^{-\beta H/2} |\sigma_i\rangle}{\sqrt{p_i}}.$$

This gives direct access to observables like hole densities and spin correlations for individual snapshots of the FHM without storing the full density matrix. Figure 1(b) shows representative METTS snapshots at different temperatures, illustrating local hole densities and spin correlations. At higher temperatures ($T \approx 0.20$), thermal fluctuations smear out strong antiferromagnetic (AFM) order, though small hole clusters are still visible. As T decreases to 0.15 and then 0.10, these clusters expand and the AFM domains become more pronounced, underlining the strong tendency of holes to aggregate and spins to form staggered patterns. Al-

though a robust stripe pattern does not fully crystallize at these temperatures, the real-space snapshots in Fig. 1(b) highlight the system's proximity to both charge and spin ordering instabilities. These charge fluctuations echo those seen experimentally in cuprates and other superconducting materials near and below the pseudogap crossover.

Comparison with ultracold-atom data Recently Prof. Immanuel Bloch's quantum-gas microscopy group implemented the single-band Hubbard model in a square optical lattice of fermionic ^{6}Li atoms for a broad range of dopings and temperatures [3]. The experimental data was compared with finite-temperature results from our METTS and determinant Quantum Monte Carlo (dQMC) data. We calculated the *magnetic susceptibility* χ_m, expressible in real space as

$$\chi_m = \frac{|\Omega|}{T}\sum_d \left(\frac{4}{N_d}\sum_{i\in\Omega}\Big[\langle \hat{S}^z_i\, \hat{S}^z_{i+d}\rangle - \langle \hat{S}^z_i\rangle\langle \hat{S}^z_{i+d}\rangle\Big]\right), \quad (2)$$

where $|\Omega|$ is the number of lattice sites in the region, d runs over relative displacements, and N_d is the count of site pairs $(i, i+d)$. The local spin operator is $\hat{S}^z_i = (\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow})/2$. In Fig. 2(a), both experiments and METTS calculations exhibit a pronounced maximum in χ_m, marking the onset of the pseudogap regime. As doping increases from half-filling to about 12.5%, this maximum in χ_m shifts and decreases in magnitude, signifying that AFM spin correlations weaken away from half-filling. To understand the dopant–spin interplay near this pseudogap regime, we investigate higher-order correlations, focusing on the third order connected, and normalized *dopant-spin-spin* correlator in Fig. 2(b):

$$C^{(3)}_{dss}(r,d) = \frac{4}{N_{r,d}}\sum_{i\in\Omega}\frac{\langle \hat{d}_i\, \hat{S}^z_{i+r+d/2}\, \hat{S}^z_{i+r-d/2}\rangle_c}{\langle \hat{d}_i\rangle}, \quad (3)$$

where $\hat{d}_i$ is the dopant operator at site i, and $\hat{S}^z_{i+r\pm d/2}$ are spin operators separated by the vector d. By examining short-range bonds, one sees how each dopant reshapes the local AFM order into an extended "magnetic polaron". The results reveal that for $|\delta| \lesssim 10\%$, dopants trigger substantial spin distortions extending across multiple lattice sites. At larger doping or higher temperature, $C^{(3)}_{dss}$ diminishes, reflecting that the polaronic cloud shrinks. These trends in polaronic correlations reveal new understanding of the pseudogap regime.

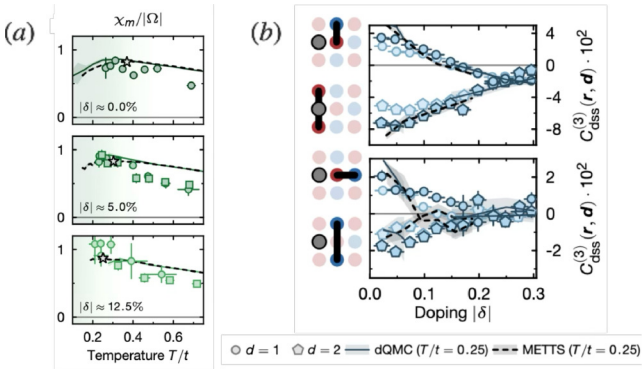

Figure 2: (a) Magnetic susceptibility χ_m vs temperature at half-filling, 5% doping, and 12.5% doping. The solid and dashed lines depict data from dQMC and METTS, respectively, and the star indicates the maximum χ_m in the METTS data. (b) Polaronic three-point connected correlator $C^{(3)}_{dss}(r,d)$ on selected bonds (nearest neighbors $|d| = 1$ and next-nearest neighbors $|d| = 2$) as a function of doping. Dark (light) blue circles correspond to temperature $T \approx 0.25$ ($T \approx 0.40$). Solid and dashed lines denote numerical simulations (dQMC and METTS, respectively).

Outlook We employed advanced tensor network simulations to understand the thermal phase diagram of the two-dimensional Fermi-Hubbard model, with emphasis on the parameter regimes where pseudogap and strange-metal physics are known to occur. At intermediate temperatures, hole clustering and antiferromagnetic (AFM) domains emerge, while lower temperatures lead to stripe order [1]. Our findings reinforce that short-range AFM correlations play a pivotal role in the pseudogap regime and simultaneously encourage the formation of charge clusters. Local doping inhomogeneities create nearly half-filled AFM islands that open a gap in the electronic spectrum. Meanwhile, surrounding hole-rich metallic regions provide low-energy states that partially fill this gap, lowering the density of states at the Fermi level without generating a full gap—a hallmark of the pseudogap regime. Together with our ongoing collaboration with cold-atom experimentalists, we also probe higher-order spin–charge correlators in the pseudogap region of the Hubbard model, shedding light on how doped holes disrupt AFM order and drive emergent phenomena.

[1] A. Sinha and A. Wietek, *Forestalled Phase Separation as the Precursor to Stripe Order*, arXiv:2411.15158 (2024).

[2] A. Wietek, Y.-Y. He, S. R. White, A. Georges, and E. M. Stoudenmire, *Stripes, Antiferromagnetism, and the Pseudogap in the Doped Hubbard Model at Finite Temperature*, Phys. Rev. X **11**, 031007 (2021).

[3] T. Chalopin *et al.*, *Probing the Magnetic Origin of the Pseudogap using a Fermi-Hubbard Quantum Simulator*, arXiv:2412.17801 (2024).

2.10 Discovering fragmented condensates in striped superconductors

NICCOLO BALDELLI, HANNES KARLSSON, AND ALEXANDER WIETEK

Strongly correlated electrons can give rise to a broad variety of intriguing emergent orders. In the context of high-temperature superconductivity, a charge density wave (CDW) refers to a state where the electron density is periodically modulated over the crystal lattice and is observed close to superconducting states in many compounds. Novel insights by several groups [1] including ours [2, 3] now arrive at the conclusion that superconductivity and CDWs can, in fact, coexist and form a state which is also referred to as a supersolid. Two of the group's studies have now unraveled an exciting phenomenon. Using unbiased numerical simulations of microscopic models we find that in the supersolid case, the condensate is "fragmented". Moreover, we gave a phenomenological explanation by proposing a simple Ginzburg-Landau theory for which we discovered novel solutions describing the individual fragments of the condensate.

Fragmented Cooper Pair Condensation in Striped Superconductors In a first paper [2] we investigated the interplay between superconductivity and a CDW using the two-dimensional t-t'-J model, a simplified theoretical framework for describing the behavior of strongly correlated electrons in high-temperature superconductors. In conventional superconductors, Cooper pairs of electrons condense into a single macroscopic quantum state. More precisely, this means that a single dominant eigenvalue in a properly defined two-particle density matrix of the form,

$$\rho_2(\boldsymbol{r}_i\sigma_i, \boldsymbol{r}_j\sigma_j|\boldsymbol{r}_k\sigma_k, \boldsymbol{r}_l\sigma_l) = \langle c^\dagger_{\boldsymbol{r}_i\sigma_i} c^\dagger_{\boldsymbol{r}_j\sigma_j} c_{\boldsymbol{r}_k\sigma_k} c_{\boldsymbol{r}_l\sigma_l}\rangle, \quad (1)$$

scales with the number of particles and, hence, signals the formation of a condensate. This definition of a condensate is also referred to as the Penrose-Onsager criterion. However, our study using the density matrix renormalization group (DMRG) now discovered that in the presence of a CDW not a single but multiple eigenvalues become dominant. As shown in Fig. 1, we observe exactly one condensate fragment per charge stripe in the system.

The corresponding eigenvectors, which are referred to as the macroscopic wave functions of the Cooper pair, also exhibit a fascinating structure. The leading eigenvector exhibits a uniform d-wave symmetry. However, the subleading wave functions then modulate this uniform pattern periodically with a certain momentum. We interpret this as Cooper pairs tunneling between the stripes and indeed forming an emergent array of Josephson junctions. As shown in Fig. 2, the individual fragments then resemble pair-density waves, i.e. superconducting states with a periodic modulation of the superconducting order parameter.

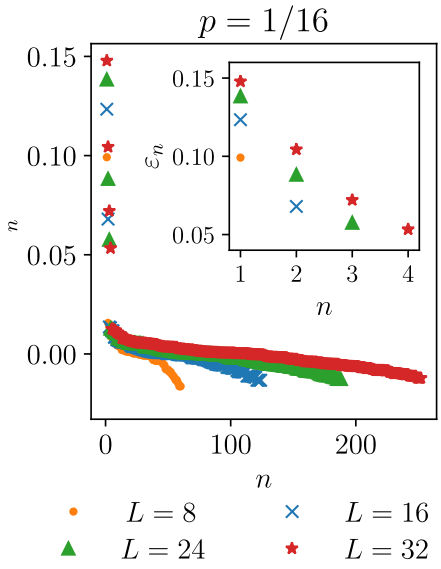

Figure 1: Spectrum of the two-body reduced density matrix $\rho_2(\boldsymbol{r}_i\sigma_i, \boldsymbol{r}_j\sigma_j|\boldsymbol{r}_k\sigma_k, \boldsymbol{r}_l\sigma_l)$ for interaction parameters of the t-t'-J model on a 32×4 cylinder when superconductivity coexists with a charge density wave. The multiple dominant eigenvalues constitute the fragments of the condensates. We observe that for system lengths $L = 8, 16, 24, 32$ the number of fragments exactly matches the number of charge stripes in the system.

In the context of Bose-Einstein condensates, fragmentation has been reported experimentally but has not been widely discussed in the context of superconductivity. The study establishes that fragmented superconductivity arises naturally in these systems, offering new insights into how CDWs and superconductivity coexist.

Even though the Penrose-Onsager criterion for superconductivity is an established method theoretically, it has recently only been applied by few groups as conventionally diagnosing off-diagonal long-range order has been preferred. With the study, we show that the additional information contained in the full two-particle density matrix can yield a plethora of additional information not contained in simple correlation functions alone.

Novel solutions in an intertwined Ginzburg-Landau Theory Building upon the findings of our first paper, the second study [3] extends the exploration of fragmented superconductivity in an extended Hubbard model, a more accurate microscopic description of processes occurring in high-temperature cuprate superconductors. We confirmed that fragmentation persists in the Hubbard model and extended system sizes. Importantly, we also develop a simple phenomenological picture explaining the emergence of multiple condensates.

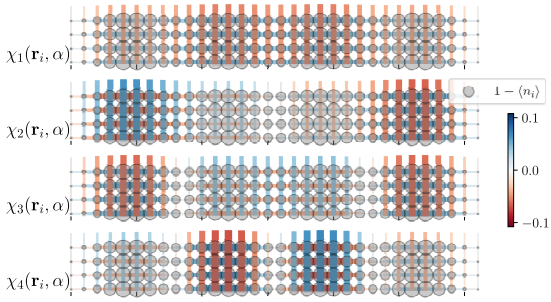

Figure 2: Macroscopic wave functions on a 32×4 cylinder corresponding to the fragments of the condensate. The size of the grey background circles depicts the local hole density exhibiting a charge density wave. The four distinct wave functions shown correspond to the four leading eigenvalues in Fig. 2. We observe that a uniform d-wave pattern is modulated with different momenta reminiscent of a pair-density wave.

To this end, we proposed an effective intertwined Ginzburg-Landau (GL) theory with a free energy density of the form,

$$\mathcal{F}[\psi] = \alpha(\boldsymbol{r})|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*}\left|\left(-i\hbar\vec{\nabla} + 2e\boldsymbol{A}\right)\psi\right|^2. \tag{2}$$

Here, we assumed that the superconducting order parameter directly couples to a periodically modulated charge density via a position-dependent parameter $\alpha(\boldsymbol{r}) = \alpha n_h(\boldsymbol{r})$, where $n_h(\boldsymbol{r})$ denotes the hole density at position $\boldsymbol{r}$. Under this assumption, we demonstrate that the intertwined GL theory admits Bloch-wave-like solutions, cf. Fig. 3, which are then compared to the macroscopic wave functions obtained via DMRG. In fact, we used the electron density distribution from DMRG as an input to the intertwined GL theory. The agreement has been found to be excellent and every fragment of the condensate can be matched with one particular solution of the intertwined GL theory.

The study also incorporates the effects of external magnetic fields. A key prediction of our theory is that superconducting vortices align with the CDW stripes. This coupling between CDWs and the superconducting condensate creates an emergent system resembling an array of Josephson junctions, where the condensates on each stripe interact via a Josephson coupling mechanism.

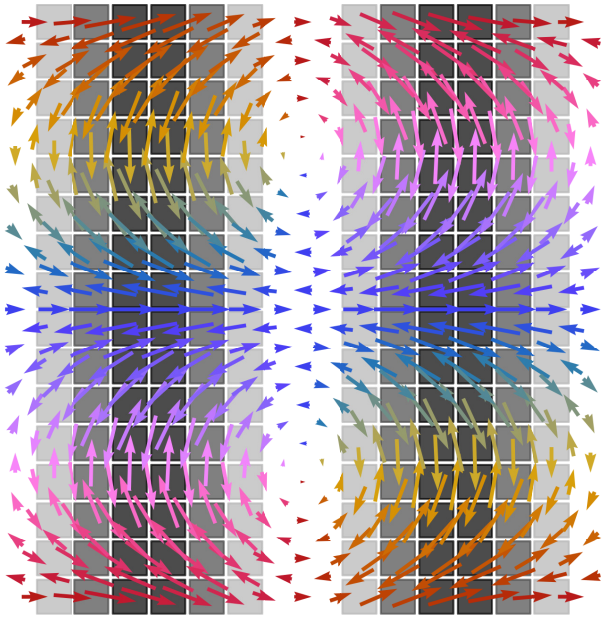

Figure 3: Solution of the proposed intertwined Ginzburg-Landau theory in the presence of two charge stripes. We find two stable solutions corresponding to two distinct condensate fragments. A key experimental signature of the supersolid phase is the pinning of vortices between the stripes of the charge density wave.

Summary Together, these studies offer a comprehensive theoretical and computational foundation for understanding supersolids in strongly correlated electron systems, i.e. a coexistence of a CDW with superconductivity. Moreover, we showed that the phenomenon is not limited to specific models but fragmentation remains a robust feature of systems with intertwined CDW and superconducting order. Importantly, the findings align with experimental observations of unconventional superconductors, such as pair-density waves in cuprates and heavy fermion materials.

The papers also propose experimental signatures of fragmented superconductivity, such as pinned vortices aligned with CDW stripes, which could be observed using scanning tunneling microscopy or Josephson tunneling spectroscopy. These predictions could guide future experiments and deepen our understanding of high-temperature superconductors.

[1] H. Xu, C.-M. Chung, M. Qin, U. Schollwöck, S. R. White, and S. Zhang, Science, Vol 384, Issue 6696 (2024)

[2] A. Wietek, Phys. Rev. Lett. **129**, 177001, Editor's suggestion (2022).

[3] N. Baldelli, H. Karlsson, B. Kloss, M. Fishman, A. Wietek, npj Quantum Materials, accepted (2025), arXiv:2307.11820

2.11 Time-dependent two-photon processes

SAJAD AZIZI, ULF SAALMANN, AND JAN M. ROST

Interaction of matter with shaped or short laser pulses exchanging two VUV photons features intricate dynamics and its control since both, time-dependence through the pulse, as well has energy-dependence through the photons' energy are externally determined parameters which can have a joint, significant influence on the dynamics with surprising effects. Controlling intense VUV pulses has only become feasible recently through seeded free electron laser (FEL) sources. Two effects we discuss here: (i) A recent experiment [2] demonstrating population control of Autler-Townes doublet levels in the continuum and control of the transfer of population to bound versus continuum states as predicted [1] through changing the chirp of a VUV pulse requiring two-photon processes. (ii) Ionizing a negative ion with a short laser pulse, sufficiently intense to initiate two photon processes, results in a peculiar variant of the photoeffect: for different photon energies a photo electron peak will appear at the same energy in the continuum [3].

Rapid adiabatic passage is a well established single-photon mechanism to transfer population from one quantum state to another with almost 100 % efficiency using a chirped pulse where the photon energy is resonant with the energy difference of the two states. Population inversion, that is, transfer to the other bound state, can be achieved independently of the chirp direction in weak fields. Using intense XUV laser pulses for this scenario, two-photon transitions become possible and in turn ionization. As we have demonstrated in [1], the ratio between transfer of population to a bound state and to the continuum depends now sensitively on the direction of the laser chirp.

This finding has motivated a recent experiment at the FERMI FEL in Trieste to realize the effect and to prove in general that one can control electronic processes with shaped laser pulses also in the VUV domain. By monitoring the photo electrons resulting from shining a chirped light pulse onto a helium gas target it could be shown that indeed, one can control the population of the individual states of the Autler-Townes split doublet via changing the chirp (ig. 1). components. Strong driving in the VUV renders the ionization non-perturbative changing the ratio in the doublet (Fig. 1). This has the consequence that in the VUV regime, the degree of ionization, that is the electron spectrum integrated over the photo electron energies (Fig. 2), depends now on the chirp strength and sign, as predicted [1]. experiment it was sufficient to propagate the time-dependent Schrödinger equation (TDSE) for a single-active electron (SAE) model of Helium which could be done numerically fast enough to also incorporate experimental broadening effects (Fig. 1). The modelled chirp rate a in the time-dependent frequency $\omega(t)$ with $d\omega/dt = at$ is linked to the experimental Φ_2 (group delay dispersion GDD) through $a = \Phi_2/(\Phi_2^2 + T^4)$, where $T = T_0/(\sqrt{2}\ln 2)$ with the Fourier-transform-limited pulse length T_0.

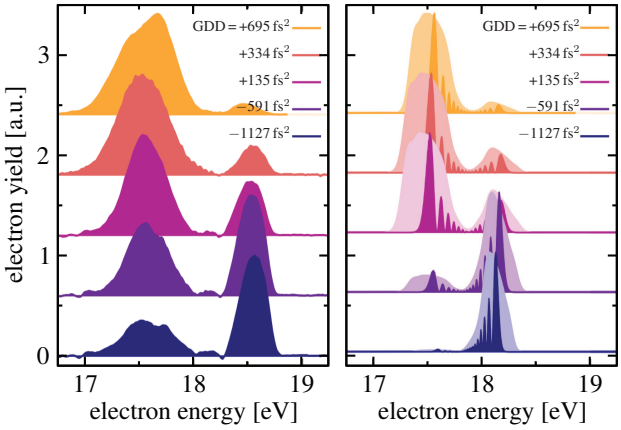

Figure 1: Photoelectron spectra in arbitrary units obtained for phase-shaped XUV pulses (see labels for GDD values; (resonant) photon energy = 21.25 eV; I_{eff} = 2.8(2) × 10^{14}W/cm^2). The control of the dressed-state populations is directly reflected in the relative change of amplitude in the photoelectron bands. The small peak at 18.13 eV results from imperfect removal of the lower intensity contribution from the aberrated focus. b, Calculations of the time-dependent Schrödinger equation for a single active electron (TDSE-SAE) and a single laser intensity corresponding to the experimental I_{eff} = 2.8 × 10^{14}W/cm^2 (dark colours). Spectral fringes reflect here the temporal progression of the Rabi frequency during the light–matter interaction. The photoelectron spectra filled with light colors account for experimental broadening effects caused by the focal intensity averaging and the instrument response function. Taken from [2].

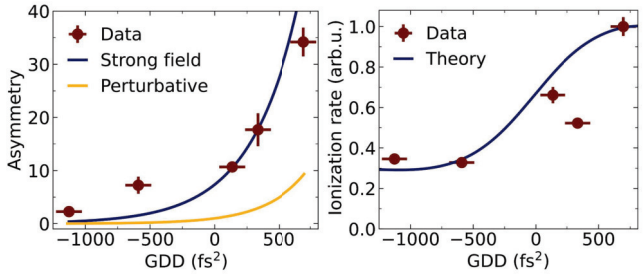

Figure 2: Left: Amplitude ratio between upper/lower photoelectron bands shown in Fig. 1. Experiment (red), full TDSE-SAE model (blue) and with the continuum treated perturbatively (yellow). Right: Dependence of the helium ionization rate on the spectral phase of the driving field from experiment (red) and the TDSE-SAE model (blue). Taken from [2].

Our second example, the zero-energy photo effect (ZEPE) features a peak near threshold ("zero energy") in the photo electron spectrum whose position does not depend on the photon energy, but on the pulse duration in sharp contrast to the standard photo ef-

fect. ZEPE is enabled by a two-photon process, where a bound electron first absorbs a photon and then emits a photon, ending again in a bound state. Only, if the laser pulse is short enough that the spectral peak at the final negative energy "leaks" into the continuum, see Fig. 3, this process becomes visible in form of photo-electrons. The leakage is suppressed for small photo electron energies, if the photo electron yield vanishes at threshold, which is the case for photo electron detachment, where a negative ion fragments into a neutral core and the electron lacking mutual long range interaction. The ZEPE effect requires pulses short enough such that their spectral bandwidth ΔE is larger than the binding energy $E_{\rm EA}$ of the detached electron, typically of the order of a few femtoseconds, conditions not realizable in ATI detachment experiments with 800 nm light. In addition, the second ionization potential should be larger than the photon energy. This suggests negative ions as ideal candidates for corresponding experiments.

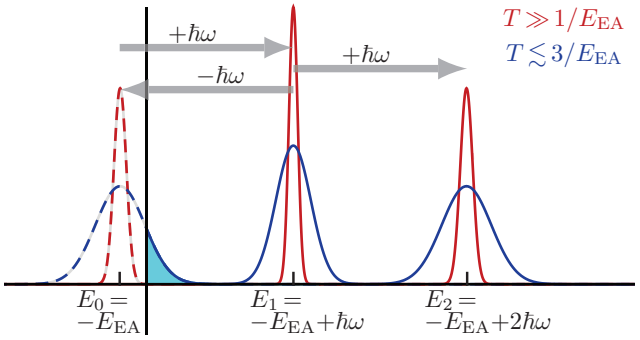

Figure 3: Multi-photon detachment of a an electron, weakly bound by electron affinity $E_{\rm EA}$ to an ion, will give rise to peaks in the photo-electron spectrum at energies $E=-E_{\rm EA}+n\omega$, shown here for n=1, 2. However, following absorption of the 1st photon it is more likely that a 2nd photon is not absorbed but emitted ($-\hbar\omega$) since the bound-continuum $|E_0\rangle\to|E_1\rangle$ transition dipole is much stronger than continuum-continuum $|E_1\rangle\to|E_2\rangle$ transition dipole. This process with net-zero energy absorption becomes only visible in the spectrum for very short pulses (blue) leading to a broad peak at $-E_{\rm EA}$ whose tail reaches into the continuum (light-blue-shaded), but not for longer pulses (red).

To understand how ZEPE comes about qualitatively and quantitatively, we take a closer look at the near-threshold energy range with the spectra of Fig. 4 for different pulse durations T and photon energies ω. One immediately sees that the spectra depend on T, but not on ω, as already anticipated. The Wigner threshold law states that for break-up of two fragments under short-range forces, the ionization probability near threshold is given by the available continuum states in momentum space, i.e.,

$$P(E\to 0) \propto \int \mathrm{d}p\, p^{2(\ell+1)}\delta(p^2/2-E) \propto E^{\ell+1/2},$$

where ℓ is the angular momentum of the fragment pair. Following the intuition that ZEPE originates in the combination of the Wigner law and a Gaussian energy distribution induced by the short laser pulse, located at the binding energy $-E_{\rm EA}$ due to the two-photon zero-energy process, the detachment probability should be given by

$$P^{\ell,\beta}_{\rm ZEPE}(E) = P_*(E)\, s_{\ell,\beta}(E/E_{\rm EA}), \tag{1}$$

$$P_*(E) = [1+E/E_*]^{-1} \tag{1a}$$

$$s_{\ell,\beta}(x) = \beta^4 x^{\ell+\frac{1}{2}} \exp(-\beta^2[x+1]^2). \tag{1b}$$

The universal shape $s_{\ell,\beta}(x)$ of the zero-energy photo-electron spectrum is fully determined by the angular momentum ℓ of the photo-electron and $\beta = E_{\rm EA}/\Delta E$ the ratio of electron affinity $E_{\rm EA}$ to spectral pulse width ΔE. From the spectral representation of the pulse and the fact that ZEPE is a two-photon process follows $\Delta E = 2/T$, which is confirmed by 2nd-order perturbation theory. Furthermore, $P_*(E)$ takes care of the slowly-varying background, which is different for each ion.

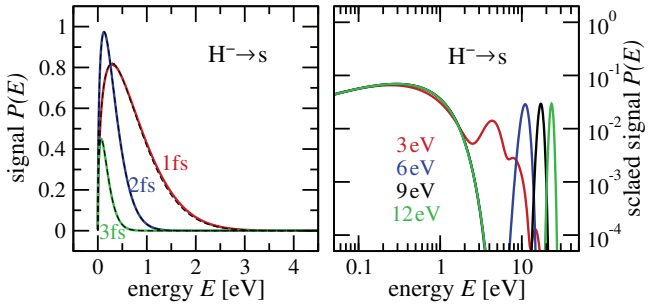

Figure 4: (a) Photo-electron spectrum of H^- for the s-channel (colored solid lines) and a Gaussian pulse of intensity $I = 10^{14}$ W/cm^2. Panel (a) features different pulse duration $T_{\rm fwhm}$=1, 2, 3 fs, for the same carrier frequency ω=9 eV; the black dashed lines are fits according to Eq. (1). Panel (b) features different photon frequencies $\omega = 3, 6, 9, 12$ eV for the same pulse length $T_{\rm fwhm} = 1$ fs in logarithmic scale. Note, that higher-order ATI peaks (at energies $E \gtrsim 6$ eV) shift with increasing ω to higher energies, while the zero-peak position ($E_{\rm peak} \approx 0.3$ eV) is independent of ω. Spectra are scaled to agree for $E = 0.1$ eV.

We close with an estimate for the number of ZEPE electrons per shot one could detect in an experiment,

$$N_{\rm exp} = N_{\rm ion}\left[I_{\rm exp}/10^{14}{\rm W/cm}^2\right]^2 P_T,$$

where $N_{\rm ion}$ is the number of ions in the target volume, $I_{\rm exp}$ the experimental laser intensity and P_T is given in the table.

Table 1: Total ionization probability P_T for H^- and O^- for accessible angular momentum channels and three pulse durations $T_{\rm fwhm}$.

$T_{\rm fwhm}$	$H^-\to s$	$H^-\to d$	$O^-\to s$	$O^-\to d$
1fs	8.9×10^{-4}	1.5×10^{-6}	1.8×10^{-4}	7.1×10^{-8}
2fs	4.4×10^{-4}	9.1×10^{-8}	3.1×10^{-6}	9.7×10^{-11}
3fs	1.1×10^{-4}	6.4×10^{-9}	3.9×10^{-8}	6.8×10^{-13}

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2.12 Intense pulse parameter scaling in extended systems

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Strong laser fields with a given peak intensity F^2 and carrier frequency ω induce typical length and momentum scales into light-matter dynamics, given by the quiver amplitude $x_0 = F/\omega^2$ and momentum amplitude $A_0 = F/\omega$. These scales unfold their effect fully when they match scales of the illuminated matter which typically requires extended targets. A prominent example is graphene, whose valley polarization is sensitive to A_0 through the distance of the Dirac points in reciprocal space [6], while high order harmonic generation (HHG) in finite periodic chains of atoms is optimized if the quiver amplitude is comparable to the length of the chain [2]. HHG from nanorods is a possible application.

In periodic systems with a band structure $E_m(\vec{k})$ in terms of the crystal momentum $\vec{k}$, a laser pulse described by its vector potential $\vec{A}(t) = \vec{A}_0 f(t)\cos\omega t$, leads in minimal coupling to a time-dependent crystal momentum $\vec{k} \to \vec{k} + \vec{A}(t)$.

Spatial scaling. We consider a chain of N atoms separated here by $d = 7$ (atomic units are used unless stated otherwise). Calculated for a specific realization and with a technique adapted from [1], HHG of the chain is shown in Fig. 1a,b. One sees an extended plateau compared to an infinite chain due to backscattering of the quivering electron wave-packet from the edges of the chain. Backscattering reverses the electron momentum, similarly as from a repulsive potential in free space (see Fig. 1c,d).

Defining N_q through $2x_q = N_q d$ we get the critical length scale of the system for efficient backscattering. Note that the quiver amplitude x_q in a band structure differs from x_0 of a free electron. However, $x_q \propto \lambda$ still holds for fixed A_0 [2]. When varying the laser wavelength λ, we indeed keep $\vec{A}_0$ fixed such that the time-dependent "trajectory" in $\vec{k}$-space remains the same. Scaling additionally the system size in order to keep $N/N_q \propto N/\lambda$ constant, one expects similar HHG spectra, which is indeed the case, see Fig. 1e. Under these conditions, the integrated harmonic yield become maximal if the full quiver amplitude and system size match $2x_q = L$, i.e., $N = N_q$ (Fig. 1f). This establishes the relevance of the light induced spatial quiver scale for delocalized electrons if their support also contains a characteristic length scale.

Such a slab of matter is prepared in F. Calegari's group in Hamburg by growing nanorods perpendicularly to a plane substrate, so that our prediction can be experimentally tested. Multiple chains with breaks of tunable size exhibit also enhanced HHG which, depending on the seize of the break, is either due to backscattering or due to an induced defect-like behavior which increases tunneling [3].

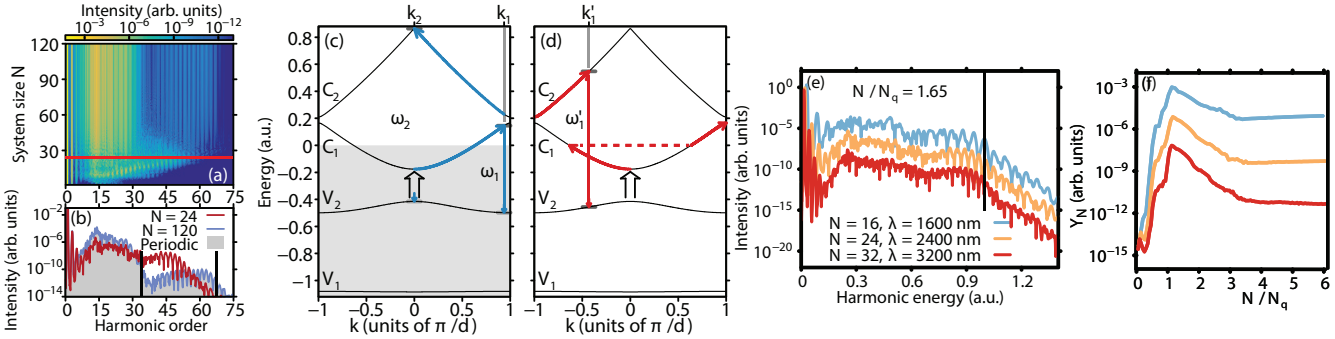

Figure 1: (a) HHG spectrum as a function of harmonic order and system size N for 2400 nm and (b) for fixed $N = 24$, indicated by the horizontal dashed lines in (a). The spectrum of the periodic system is shown as shaded area for comparison. The dashed lines indicate the estimates of the 1st and 2nd cutoff for the periodic system at ω_1 and ω_2, see (c), which gives a sketch of the k-space dynamics in the periodic system, for an electron excited to the bottom of first conduction band at $A(t_0) \approx -A_0$. The maximal energy differences between the first conduction and second valence band or the second conduction and valence band (i. e., the cutoffs ω_1 and ω_2) are achieved at $k_1 = 2A_0$ and $k_2 = 0$. Panel (d) sketches the k-space dynamics in the finite system, with an edge backscattering event in the first conduction band at the vacuum level occurring at $A(t_s) = -A_0$. The horizontal dotted line represents the sign change of $k(t)$ due to backscattering. With a subsequent band-gap transition to the seocond conduction band, the path corresponds to the maximally achievable harmonic energy in the backscattering case ω_1' at k_1'. Panel (e) presents HHG spectra as a function of photonenergy and (f) their integrated yield beyond the first cutoff ω_1 as a function of scaled system size N/N_q. The vertical dashed line in panel (d) indicates the edge-backscattering cutoff at ω_1'. In all calculations $A_0 = 0.21$ was used; adapted from [2].

Momentum scaling. Apart from the standard reciprocal lattice constants for periodic systems, graphene and similar two-dimensional systems have another characteristic momentum vector $\vec{\Delta}$ connecting the two Dirac points in the unit cell (see Fig. 2, which reveals that there are two more equivalent vectors rotated by ± 120 degrees). The Dirac points play an important role for valley polarization η which describes the imbalance

$$\eta = (P_K - P_{K'})/(P_K + P_{K'}) \tag{1}$$

of electron density P_K and $P_{K'}$ excited from electrons around $\vec{K}$ and $\vec{K}'$, respectively, relative to the total excitation $P_K + P_{K'}$. The selective excitation may be achieved by tailored light pulses. For a long time it was thought that one needs laser pulses with a rather complicated circular polarization with two colors ω and 2ω [4]. However, one can achieve even larger η realizing a particular "resonance" condition, namely if the peak vector potential $\vec{A}_0 \approx \vec{\Delta}$ implying linear polarization along $\vec{\Delta}$. In addition, suitable pulses must avoid $\vec{A}_0 \approx -\vec{\Delta}$, which would undo the transfer of electron density to the other valley. This requires multiharmonic pulses [5], or in the simplest case, a close-to-half cycle pulse [6], as can be seen in Fig. 3.

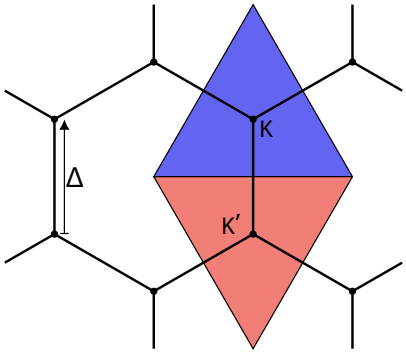

Figure 2: Sketch of the triangular domains in reciprocal space around $\vec{K}$ and $\vec{K}'$ with momentum scale Δ indicated; adapted from [5].

Of interest in the present context is that all suitable pulse forms deliver the largest valley polarization at "resonance", i.e. $A_0 \approx \Delta$ as Fig. 3 also shows. From understanding the mechanism behind valley polarization with linearly polarized pulses [6], one can devise dedicated pulse shapes which generate even higher η. To this end we have proposed a pulse which contains a pedestal $f(t) = S_{T_1}(t) + S_{T_2}(t)$, where

$$S_T(t) = \tfrac{1}{2}\exp(-2\ln 2\, t^2/T^2). \tag{2}$$

As can be seen in Fig. 3a it performs with $T_2 = 8\,T_1$ significantly better than the pristine half-cycle pulse and is accompanied by the lowest ionization (see Fig. 3b) which is important for minimal damage to the device.

One might ask to what extent these findings can be transferred to materials with gaps, most notably graphene on substrates. Interestingly, the pulse shape maximizing valley polarization η remains the same for moderately gapped graphene (Fig. 4). This implies that the resonance condition $A_0/\Delta \approx 1$ prevails also in this situation and therefore renders the strong field scaling A_0 in reciprocal space of pertinent relevance.

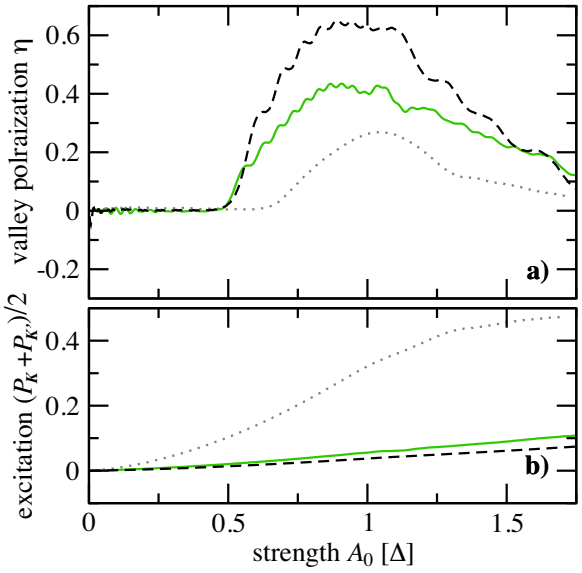

Figure 3: (a) Valley polarization and (b) excitation as a function of the scaled peak vector potential A_0/Δ for half-cycle pulses with $\lambda = 7.2$, μm (green), 2.4 μm with additional pedestal with $T_2 = 8\,T_1$, $T_1 = T_\omega/5$ with $T_\omega = 2\pi/\omega$ (dashed), and the two-color pulse from [4] (dotted); adapted from [6].

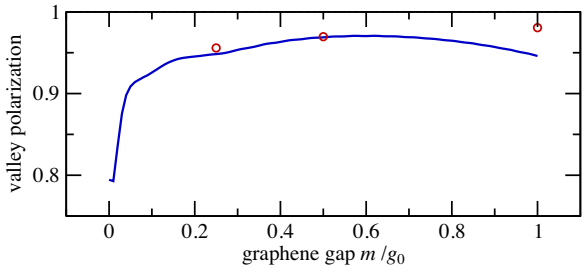

Figure 4: Valley polarization as function of the gap m in units of the hopping integral g_0 in two-band graphene [6]. The line shows valley polarization η with the pulse shape optimized numerically for $m = 0$ in the parameters A_i, ω_i, T_i and ϕ_2 with $\phi_1 = 0$ for the anlytical form $\vec{A}(t) = \hat{z}[\sum_{i=1,2} A_i S_{T_i}(t)\cos(\omega t + \phi_i)]$ with $S_T(t)$ from (2). The optimized pulse is very close to the analytical half-cycle pulse with a pedestal as discussed. The red circles are VPs with pulses numerically optimized at the respective m/g_0.

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2.13 Dyadic approach to multidimensional spectroscopy

XING GAO, LIPENG CHEN, AND ALEXANDER EISFELD

The stochastic quantum state diffusion (QSD) provides a powerful way to solve the dynamics of open quantum systems with a structured non-Markovian environment [1]. An outstanding problem is how to implement perturbative schemes, as commonly used for example in multidimensional femtosecond spectroscopy. In the recent years we have developed such a perturbative scheme for the non-Markovian quantum state diffusion (NMQSD) [2,3] and implemented it within the framework of an adaptive version of the hierarchy of pure states (HOPS). We calculate third order optical response functions for systems consisting of hundreds of molecules [4].

We consider a molecular aggregate composed of N interacting molecules, where each molecule is described by two electronic levels, the electronic ground state $|g_n\rangle$ and the electronic excited state $|e_n\rangle$, $n = 1, \cdots, N$. The system Hamiltonian can then be written as

$$\hat{H}_{\rm S} = \sum_{n=1}^{N} \epsilon_n \hat{\sigma}_n^\dagger \hat{\sigma}_n + \sum_n \sum_{m\neq n} V_{nm} \hat{\sigma}_n^\dagger \hat{\sigma}_m \qquad (1)$$

where ϵ_n is the energy required to excite the $n^{\rm th}$ molecule, V_{nm} is the electronic coupling between excited molecules n and m, and $\hat{\sigma}_n = |g_n\rangle\langle e_n|$. For third-order two-dimensional (2D) spectroscopy, we need the common ground state $|g\rangle = \prod_{n=1}^{N} |g_n\rangle$, singly excited states $|n\rangle = \hat{\sigma}_n^\dagger |g\rangle$, and doubly excited states $|nm\rangle = \hat{\sigma}_n^\dagger \hat{\sigma}_m^\dagger |g\rangle$, $n < m$.

In a 2D spectroscopy experiment, the system interacts with three laser pulses at controlled inter-pulse delay times. The electric field is written as $\mathbf{E}(\mathbf{r}, t) = \sum_{a=1}^{3} \mathbf{e}_a E_a(t-t_a) e^{i\mathbf{k}_a\cdot\mathbf{r} - i\omega_a(t-t_a)} + \text{H.c.}$, with $\mathbf{e}_a$, $\mathbf{k}_a$, ω_a, $E_a(t)$, and t_a denoting the polarization unit vector, the wave vector, the carrier frequency, the envelope, and the central time of the ath pulse, respectively. The field-matter interaction Hamiltonian is

$$\hat{H}_{\rm F}(t) = -\hat{\boldsymbol{\mu}} \cdot \mathbf{E}(\mathbf{r}, t), \qquad (2)$$

where $\hat{\boldsymbol{\mu}}$ is the total transition dipole operator $\hat{\boldsymbol{\mu}} = \sum_{n=1}^{N} \boldsymbol{\mu}_n (\hat{\sigma}_n + \hat{\sigma}_n^\dagger)$ and $\boldsymbol{\mu}_n$ is the transition dipole moment of molecule n.

We write the $M^{\rm th}$ order response function as

$$R\begin{bmatrix} \tau_1, \ldots, \tau_M \\ \hat{v}_1^K, \ldots, \hat{v}_M^K \\ v_1^B, \ldots, v_M^B \end{bmatrix} = \mathrm{Tr}\Big\{ \hat{F}\, \hat{\rho}^{(M)} \begin{bmatrix} \tau_1, \ldots, \tau_M \\ \hat{v}_1^K, \ldots, \hat{v}_M^K \\ \hat{v}_1^B, \ldots, \hat{v}_M^B \end{bmatrix} \Big\} \qquad (3)$$

where the expectation value of an observable $\hat{F}$, in our case $\hat{F} = \hat{\boldsymbol{\mu}}$, is calculated with respect to a density matrix that is obtained in $M^{\rm th}$ order of perturbation theory. The parameters in the rectangular brackets track the order of interactions influencing the *ket* (row 2) vs *bra* (row 3) time evolution associated with a particular time-correlation function. The first row contains the intervals $\tau_i = t_{i+1} - t_i$ between interaction at time t_i and the following interaction. The last interval τ_M contains the final time t of the evolution, i.e., $\tau_M = t - t_M$. The sequences of operators in the second and third row identifies the operators acting on the *bra* and *ket* side (respectively) at each interaction time and thereby define a specific response function. We use the short-hand $\hat{\rho}^{(M)} = \hat{\rho}^{(M)}\begin{bmatrix} \tau_1, \ldots, \tau_M \\ \hat{v}_1^K, \ldots, \hat{v}_M^K \\ \hat{v}_1^B, \ldots, \hat{v}_M^B \end{bmatrix}$, where the $M^{\rm th}$ order density matrix is recursively defined by

$$\hat{\rho}^{(j)} = \hat{U}(\tau_j)\, \hat{v}_j^K\, \hat{\rho}^{(j-1)} \big(\hat{v}_j^B\big)^\dagger \hat{U}^\dagger(\tau_j) \qquad (4)$$

with $\hat{U}(\tau)$ is the time-evolution operator of the system without the electromagnetic field. The operators $\hat{v}_j^{\rm K}$ act always on the *ket* side and the operators $\hat{v}_j^{\rm B}$ always on the *bra* side of $\hat{\rho}$. An important constraint is that for each pair $\hat{v}_j^{\rm K}$, $\hat{v}_j^{\rm B}$, with the same index j one of the corresponding operators is the unit operator (which we denote by $\mathbb{I}$). Explicitly we have $\hat{v}_j^{\rm K} = \hat{V}_j$, $\hat{v}_j^{\rm B} = \mathbb{I}$ or $\hat{v}_j^{\rm K} = \mathbb{I}$, $\hat{v}_j^{\rm B} = \hat{V}_j$ with $\hat{V}_j = \hat{H}_{\rm F}(t_j)$.

We aim at a description using stochastic wavefunctions. To this end we double the system's Hilbert space and introduce states $|\widetilde{\psi}(t, \mathbf{z})\rangle = \begin{pmatrix} |\phi_{\rm B}(t, \mathbf{z})\rangle \\ |\phi_{\rm K}(t, \mathbf{z})\rangle \end{pmatrix}$ that contain bra and ket contributions of the density matrix. These states are evolved according to

$$|\widetilde{\psi}(t)\rangle = \widetilde{\mathcal{U}}(\tau_M, \mathbf{z}) \widetilde{V}_M \cdots \widetilde{\mathcal{U}}(\tau_1, \mathbf{z}) \widetilde{V}_1 |\widetilde{\psi}(0)\rangle, \qquad (5)$$

with initial state $|\widetilde{\psi}(0)\rangle = \big(|\phi_{\rm ini}\rangle, |\phi_{\rm ini}\rangle\big)^T$ and interaction operators $\widetilde{V}_j = \begin{pmatrix} \hat{v}_j^{\rm B} & 0 \\ 0 & \hat{v}_j^{\rm K} \end{pmatrix}$. The time evolutions $\widetilde{\mathcal{U}}(\tau_j, \mathbf{z}^*)$ between the interactions $\widetilde{V}_j$ is obtained from the stochastic NMQSD equation

$$\begin{aligned} \partial_t |\tilde{\psi}(t, \mathbf{z})\rangle &= (-i\widetilde{H}_{\rm S} + \textstyle\sum_n \widetilde{L}_n\, \zeta_n(t, \mathbf{z})) |\tilde{\psi}(t, \mathbf{z})\rangle \\ &\quad - \textstyle\sum_n \Big(\widetilde{L}_n^\dagger - \langle \widetilde{L}_n^\dagger \rangle_t \Big) \int_0^t \mathrm{d}s\, \alpha_n(t-s) \frac{\delta |\tilde{\psi}(t, \mathbf{z})\rangle}{\delta z_{s,n}^*}, \end{aligned} \qquad (6)$$

where $\mathbf{z}$ comprises a set of complex Gaussian stochastic processes $z_{t,n}^*$ with mean $\mathcal{M}[z_{t,n}] = 0$, and correlations $\mathcal{M}[z_{t,n} z_{s,m}] = 0$ and $\mathcal{M}[z_{t,n} z_{s,m}^*] = \alpha_n(t-s)\delta_{nm}$. Here, $\alpha_n(t)$ is the correlation function of the environment. These processes enter via $\zeta_n(t, \mathbf{z}) = z_{t,n}^* + \int_0^t ds\, \alpha_n^*(t-s) \langle \hat{L}_n^\dagger \rangle_s$, where the expectation values $\langle \cdot \rangle_t$ are calculated using the normalized state $|\tilde{\psi}(t, \mathbf{z})\rangle / \sqrt{\langle \tilde{\psi}(t, \mathbf{z}) | \tilde{\psi}(t, \mathbf{z}) \rangle}$. Furthermore, we have introduced $\widetilde{H}_S = \begin{pmatrix} \hat{H}_{\rm S} & 0 \\ 0 & \hat{H}_{\rm S} \end{pmatrix}$ and $\widetilde{L}_n = \begin{pmatrix} \hat{L}_n & 0 \\ 0 & \hat{L}_n \end{pmatrix}$.

The M^{th} order 'response function' can be calculated via

$$R^{(M)} = \mathcal{M}\{R^{(M)}(\mathbf{z})\}, \tag{7}$$

with $R^{(M)}(z) = \mathcal{I}\langle\widetilde{\psi}(t,\mathbf{z})|\tilde{F}|\widetilde{\psi}(t,\mathbf{z})\rangle$, where $\mathcal{I} = \prod_{j=1}^{M} ||\widetilde{V}_j\widetilde{\psi}(t_j,\mathbf{z})||^2/||\widetilde{\psi}(t_{j+1},\mathbf{z})||^2$.

In the following, we show calculations for a dimer ($N = 2$) consisting of identical monomers (i.e. $\epsilon_n = \epsilon$) with parallel transition dipoles ($\boldsymbol{\mu}_n = \boldsymbol{\mu}$). For the bath-correlation functions we choose a single exponential $\alpha_n(t) = \alpha(t) = pe^{-i\Omega t-\gamma|t|}$, with $p = 1.8$, $\gamma = 0.25$ and the vibrational frequency Ω as the unit of energy. This correlation function corresponds to a damped vibrational mode at zero temperature. We consider the third order response functions that contribute to 2D electronic spectroscopy. For the three time intervals between the interactions the commonly used notation τ, T, and t' is adopted (see Fig. 1A). In Fig. 1C We present plots for the ground state bleaching (GSB), stimulated emission (SE) and excited state absorption (ESA) signals.

$$\begin{aligned} S_{\text{GSB}}(\omega_\tau,T,\omega_t) &= S_3^{(-)}(\omega_\tau,T,\omega_t) + S_4^{(+)}(\omega_\tau,T,\omega_t) \\ S_{\text{SE}}(\omega_\tau,T,\omega_t) &= S_2^{(-)}(\omega_\tau,T,\omega_t) + S_1^{(+)}(\omega_\tau,T,\omega_t) \\ S_{\text{ESA}}(\omega_\tau,T,\omega_t) &= -\left(S_5^{(-)}(\omega_\tau,T,\omega_t) + S_6^{(+)}(\omega_\tau,T,\omega_t)\right) \end{aligned}$$

with $S_\ell^{(\pm)}(\omega_\tau,T,\omega_t) = \text{Re}\iint_0^\infty r_\ell(\tau,T,t)e^{\pm i\omega_\tau\tau}e^{i\omega_t t}\text{d}t\text{d}\tau$ where r_ℓ represents response functions calculated for specific choices of $\hat{\tilde{V}}_j$.

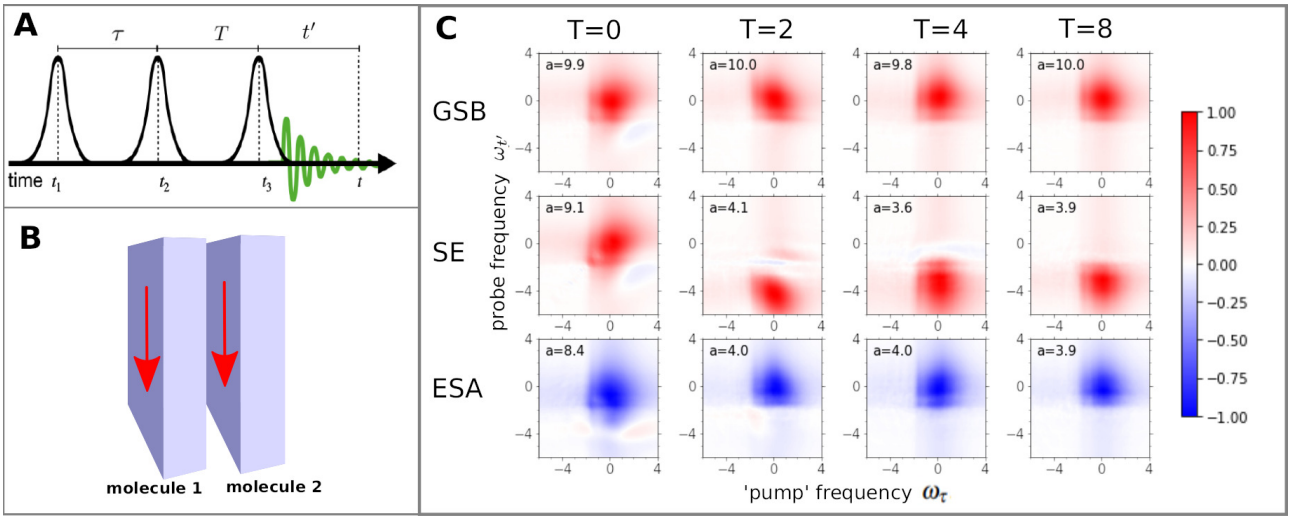

Figure 1: A: Pulse sequence for two-dimensional spectroscopy. B: Molecular dimer with parallel transition dipoles (red arrows). C: Two-dimensional spectra and their convergence properties for a dimer with two identical monomers and strong system-bath coupling ($p = 1.8$). The other parameters are $\gamma = 0.25$ and $V = 0.3$, where the energies are in units of Ω. GSB, SE and ESA spectra are shown for different waiting times T. HOPS calculations with $N_{\text{traj}} = 1000$ trajectories. For convenience, we have normalized all spectra to the maximal value $a = \max[S(\omega_\tau,\omega_t)]$, which is indicated in each panel. The spectra are in agreement with density matrix based calculations [3].

We have implemented this formalism within an adaptive scheme to solve the NMQSD equation, which is based on the powerful hierarchy of pure states (HOPS) approach, which takes advantage of the property that the noise tends to localize individual trajectories. Since the method is very fast, combining it with machine learning techniques we were able to predict the arrangement of molecules in a dimer from the experimentally measured spectra. Finally, we note that our formalism is not restricted to optical spectroscopy, but can be applied to any open quantum system interacting with external fields.

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2.14 Topological edge states in a Rydberg composite

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We examine topological phases and symmetry-protected electronic edge states in the context of a Rydberg composite: a Rydberg atom interfaced with a structured arrangement of ground-state atoms. The spectrum of the electronic Hamiltonian of such a composite possesses a mapping to that of a tight-binding Hamiltonian, which can exhibit nontrivial topology depending on the arrangement of the ground-state atoms and the principal quantum number of the Rydberg state.

The Hamiltonian of a Rydberg composite, with scatterers placed at positions $\vec{R}_q$, is (in atomic units)

$$H_\mathrm{e} = -\frac{\nabla^2}{2} - \frac{1}{r} + \sum_{q=1}^{M} 2\pi a_s \delta^3(\vec{r} - \vec{R}_q). \qquad (1)$$

The first two terms govern the electron's motion in the Coulomb field of the Rydberg core, while the last term describes its interaction with the scatterers using the Fermi pseudopotential. The interaction strength is determined by the S-wave scattering length a_s, and is too weak to mix Rydberg states with different principal quantum numbers ν. However, it splits the degenerate Rydberg levels with different angular momentum l but the same ν into two subspaces. The first, of size $\nu^2 - M$, remains degenerate and unshifted, while the second, of size M, splits away [1]. It is in this shifted manifold that topologically protected edge states can be realized.

One can transform the Hamiltonian (1) to have the structure of a tight-binding Hamiltonian [1]

$$H = \sum_{q=1}^{M} E_q |q\rangle\langle q| + \sum_{q}^{M} \sum_{q' \neq q}^{M} V_{qq'} |q\rangle\langle q'|, \qquad (2)$$

where the hopping terms $V_{qq'}$ and on-site potentials E_q are determined by the parameters of the Rydberg system – the scatterer positions and principal quantum number. The state $|q\rangle$ describes a wave function which is localized on the scatterer at position $\vec{R}_q$. In Ref. [1] we have shown that one can arrange the atoms in a way to realize one-dimensional linear chains with specific disorder allowing one to study Anderson localization.

We now discuss different arrangements that correspond to effective lattice models with topological features. Three examples are presented in Figure 1. In each case, we consider atoms arranged in a (broken) ring around the Rydberg atom, which fixes a common E_q for all scatterers. We select the number of scatterers M, the principal quantum number ν, and radius $R = R_q$ such that the desired hopping terms $V_{qq'}$ are realized. The examples shown in Figure 1 (a) and (b) realize the well-known SSH dimer and trimer chain, respectively. In the following we discuss example (c) in more detail. Here, the unit cell consists of three lattice sites, where each pair of sites within the unit cell is connected with an equal hopping amplitude u. Each triangle is coupled to its neighbor by the hopping amplitudes a (magenta), b (green), and c (cyan, dashed), as shown in Fig. 1(c)i; in general these amplitudes can all differ. We realize the corresponding Hamiltonian by the arrangement shown in Fig. 1(c)ii using a radius R_2 that is considerably smaller than the classical turning point of the Rydberg electron which is $R_1 = 2\nu^2$. In general, as the radius of the ring shrinks, the interactions become longer-ranged [1].

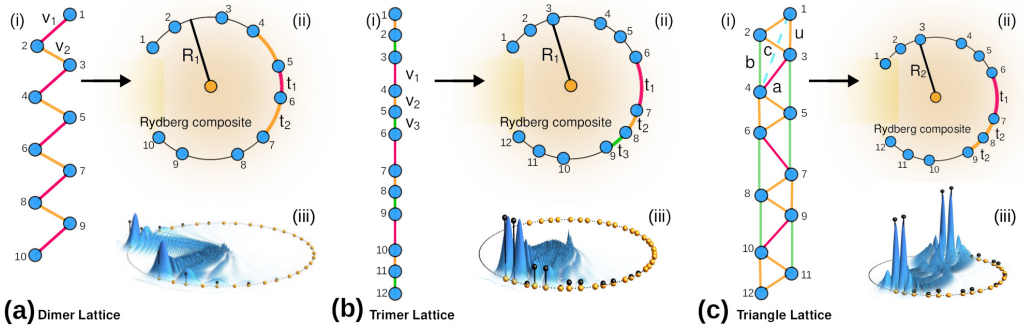

Figure 1: Schematics of the three models: (a) dimer SSH chain, (b) trimer SSH chain, and (c) triangle chain. In each panel, (i) depicts the desired tight-binding lattice and defines the couplings between sites, and (ii) sketches the Rydberg composite corresponding to this lattice. Note that (c) is realized for a smaller radius than that of (b). In (iii) examples of edge states realized in the respective arrangements. The figure is adapted from Ref. [2].

In Fig. 2, we show results for $\nu = 60$ and $R_2 = 1.74\nu^2$. In (a) the band spectrum for $M = 24$ atoms is plotted with black curves as a function of t_1. Three bands are clearly visible. The upper two repeatedly cross one another. Outside of these crossing regions, a pair of zero-energy modes is clearly present in the band gap. Between the lower two bands there are no unambiguous edge states for this small lattice, although inspection of the eigenstates for slightly larger lattice dimensions (not shown here) suggests that the states in between the two bands in the region from $0.1 < t_1 < t_2$ are indeed edge states.

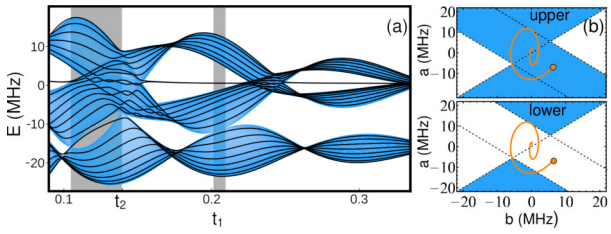

Figure 2: (a) The energy spectrum of the triangle chain Rydberg composite. The black curves show the Rydberg energies as a function of the arc-length t_1 (see Fig. 1(c)ii) for $\nu = 60$, $R = 1.74\nu^2$, and $M = 24$ scatterers. The energies are centered around the on-site potential E_q, and are plotted as a function of t_1 for fixed $t_2 = 2\pi R/45$. The blue curves show the spectrum for the same lattice parameters but $M = 300$. Topologically protected edge states are found in the middle of the upper band gap for all t_1 values, although they disappear when the bands cross as discussed in the text. One of these edge states, for $t_1 = 0.2$, is shown in Fig. 1(c)iii. The lower band gap has $\mathcal{Z} = \pi$ only within the gray shaded regions, where degenerate states in the band gap can be seen in the spectrum of the larger lattice. (b) The Zak phase of the upper and lower band gaps. Blue regions have $\mathcal{Z} = \pi$; while white regions have $\mathcal{Z} = 0$. The orange curve shows how this parameter space is traversed as we parameterically change t_1, as described in the text. The figure is taken from Ref. [2].

To analyze this spectrum, we turn to the bulk Hamiltonian, which is given by

$$H^{\text{bulk}}_{\text{triangle}}(k) = \begin{pmatrix} 2c\cos k & u + be^{-ik} & u + ae^{-ik} \\ u + be^{ik} & 2c\cos k & u + be^{-ik} \\ u + ae^{ik} & u + be^{ik} & 2c\cos k \end{pmatrix}. \quad (3)$$

Note that the coupling c enters the bulk Hamiltonian only on the diagonal, and therefore has no impact on the gap closing conditions or the topological phase transitions. The Hamiltonian is inversion-symmetric, and therefore we can characterize its topological features using the Zak phase $\mathcal{Z}$ as a quantized topological invariant. In the bottom (top) panel of Fig. 2(b), we show the phase diagram of $\mathcal{Z}$ as a function of the hopping amplitudes a and b for the lower (upper) band gap. The blue (shaded) color denotes the topological phase ($\mathcal{Z} = \pi$) and white the trivial phase ($\mathcal{Z} = 0$). The gray dashed lines show the gap closing conditions, which are sufficient but not necessary for the existence of a topological phase transition. These conditions are satisfied when $a = b$ or $b = \pm 2u - a$. We have computed the phase diagram for all a and b values in the plotted range, but as a and b depend parametrically on the arclength t_1, we cannot probe this full parameter space in the Rydberg composite. The orange curve shows the path through this parameter space that we can attain by varying t_1 over the range shown in Fig. 2a, starting at $t_1 = 0.09$ at the marker and ending at $t_1 = 0.33$. Using this curve we can analyze the states in panel (a) with respect to their topological properties. For the chosen ν, R and M, the orange curve in the upper band gap does not enter the region with a Zak phase of 0; for this reason there are always edge states visible when the bands are not overlapping. When the bands overlap, these edge states disappear even though the Zak phase remains equal to π. In contrast, the Zak phase in the bottom gap is zero except for two intervals. These correspond to the regions highlighted in Fig. 2(a) with gray boxes. Since the spectrum in panel (a) is for only a relatively small number of scatterers, the distinction between band edges and states within the band gap is not clear. Therefore, we artificially extended the system to 300 sites and plotted the resulting spectrum in blue. The edge states in the lower band gap can now clearly be seen, at least in the larger region with $\mathcal{Z} = \pi$ just below $t_1 = t_2$. We have confirmed that these are edge states by adding disorder to the system which preserves the inversion symmetry. Under this disorder, the character of these edge states is preserved.

The above examples demonstrate that with Rydberg composites one can realize Hamiltonians that exhibit a variety of interesting topological features. For the design and interpretation of the Rydberg composite we utilized the useful link between the Rydberg composite and a tight-binding Hamiltonian, which was previously elucidated in the context of Anderson localization [1].

The key ingedient of the setup discussed above is the scattering of a Rydberg electron at ground state atoms. We have used this fundamental interaction also in different contexts, for example in the coherent transfer of vibrational excitations of trapped atoms [3].

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2.15 Cavity-Polaritons via Higher-Order Van Hove Singularities

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Introduction. The emergence of a type of cavity-polariton driven by the usual presence of the Van Hove singularity (VHS) in the joint density of states (JDOS) of an insulating phase, was considered in the context of 1D nanowires [1]. The concept is that a cavity-photon coupled with an insulator phase in the energy range just below the band gap, does not suffer from absorption and experiences a hybridization with the interband particle-hole excitations, the strength of which increases with the order of the VHS singularity. Since the order of VHSs increases as the system's dimensionality is reduced, one-dimensional systems are the most obvious candidates for the implementation of this mechanism. For such systems, the singularity consists of an inverse square-root divergence [2].
However, the absence of absorption in the whole region below the band gap proves difficult to apply to all of the aforementioned solid-state platforms since either the Coulomb interactions between electrons or the presence of other degrees of freedom spoil the zero-absorption single-particle description, giving rise to collective excitations within the gap like excitons.
Guided by these insights, our research has concentrated on insulating phases realized in ultracold atom platforms, where the single-particle model is especially relevant due to the complete tunability of atom-atom interactions. Our choice of ultracold atoms is motivated not only by the potential to eliminate absorption but also by the goal of significantly enhancing dispersion. Indeed, the high tunability of optical lattices provides an alternative route to lowering dimensionality for this purpose: band engineering. This is because the ability to manipulate the band dispersions of the insulator ensures reliable access to the realm of higher-order Van Hove Singularities (HOVHS), a phenomenon previously explored primarily within the realm of two-dimensional topological materials

Van-Hove-Polariton formation. A polariton consists of a hybrid state of light and a matter excitation. Given a class of excitation states in a medium, an ideal scenario for the emergence of a long-lived polariton is one where the density of states associated with these excitations is large above a gap energy E_g and vanishes immediately below it. Consider for example a density of states that vanishes for energy values below the gap E_g and shows a divergence as the gap is approached from above. These proprieties, indeed, imply that a photon interacting with the medium, with a coupling strength g at an energy $E_\gamma \lesssim E_g$, simultaneously experiences no absorption and undergoes a hybridization that is all the more significant the larger the density of states above the gap, being indirectly influenced by the presence of the excitations. These principles apply in the absence of other types of sub-gap excitations that could spoil the zero-absorption condition. A setting of this type is potentially provided by a cavity photon coupled with the bands of an insulating phase, where interband transitions play the role of excitations and E_g corresponds to the band-gap energy. However, while the band gap ensures the absence of interband excitations below E_g, it does not guarantee that the density of states—referred to in the context of interband transitions as the joint density of states (JDOS)—is large above it. A possible way to achieve this is by tailoring the shape of the bands.

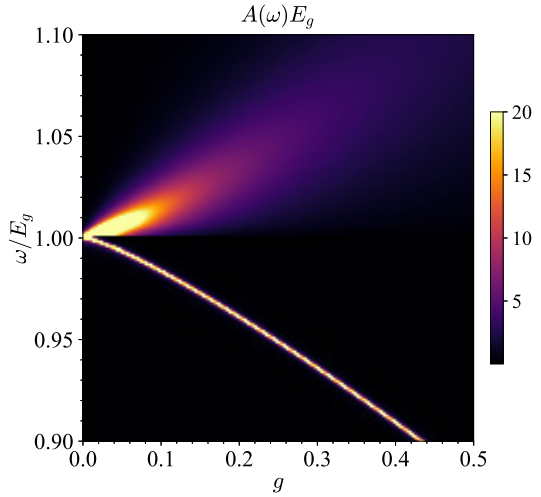

Figure 1: Spectral function $A(\omega)$ as a function of energy ω and coupling strength g, with the cavity frequency ω_c set equal to the band gap E_g. The spectrum reveals two distinct regions. For $\omega > E_g$, the spectral function exhibits broadened features dominated by absorption processes. The high density of states available for interband transitions suppresses the formation of a sharp polaritonic band, despite hybridization occurring in this regime. For $\omega < E_g$, a highly coherent lower polaritonic branch emerges, characterized by zero absorption.

In this work [3], we propose adopting this strategy in two-dimensional insulating phases realized with ultracold atoms, where band engineering is enabled by the high tunability of optical lattices. By doing so, we also access the possibility of implementing higher-order van Hove singularities (HOVHS) in ultracold atom systems. Indeed, from a mathematical perspective, modifying the band dispersion of an insulating phase can increase the order of the singularity naturally present in its JDOS at the gap, known as Van Hove Singularity (VHS). Moreover, such systems are free of sub-gap collective excitations due to the intrinsic non-disordered nature of the system and the possibility if tuning atom-atom interactions to zero. Motivated by this perspective, we identified a specific type of insu-

lating phase on a chequerboard optical lattice, which gives rise to a new type of HOVHS in the JDOS at the band-gap energy. This HOVHS arises from the dispersion of the bands near the M point that is quartic inward within the Brillouin Zone (BZ), deviating from the standard parabolic case, and remains flat along the edges of the BZ. We thus show the formation of VH-polaritons in Fig. 1, where the spectral function $A(\omega)$ is plotted as a function of ω (energy) and g (coupling strength). As the cavity frequency ω_c is tuned to the gap edge E_g, the spectrum of excitations reveals two distinct regions: one above the gap ($\omega > E_g$) and one below the gap ($\omega < E_g$). Above the gap ($\omega > E_g$), the spectral function reveals broadened features dominated by absorption processes. The high density of states available for interband transitions hinders the formation of a sharp polaritonic band, even though hybridization occurs in this regime.

Enhanced Vacuum-Rabi-Splitting. In contrast, below the gap ($\omega < E_g$), the spectral function exhibits a highly coherent lower polaritonic branch characterized by zero absorption. This branch reflects the robust hybridization between light and matter, as evidenced by its significant bending away from the cavity frequency $\omega_c = E_g$ as the coupling strength g increases. The bending of the lower polaritonic branch arises from the combined effect of the coupling strength g and the VHS: the higher the order of the singularity, the stronger the effect. This is evident from Fig. 2, where the avoided crossing (called vacuum Rabi Splitting in polaritonics), defined as the distance between the polaritonic branch $\omega_p(g)$ and the onset of the continuum at $\omega_c = E_g$, is plotted for three different types of insulators.

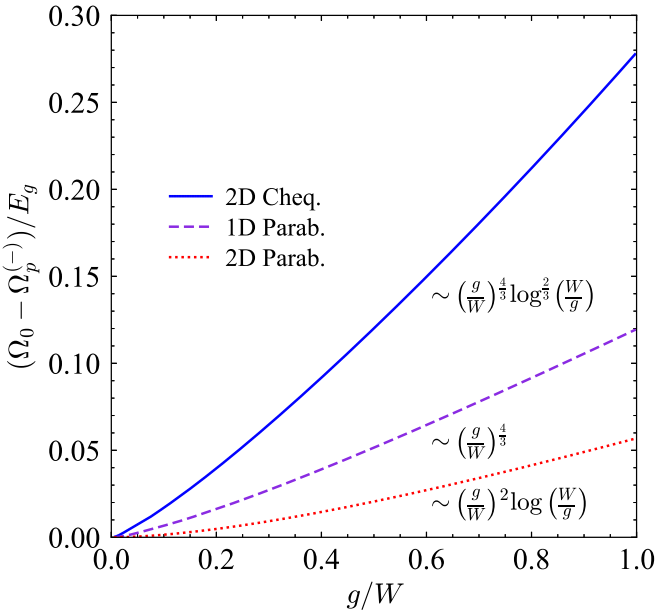

Figure 2: Lower polaritonic branch, plotted as a function of the coupling strength g, for the three cases of insulator band structures: 2D parabolic, 1D parabolic, and 2D chequerboard. For the 2D parabolic case, the energy shift $(E_g - \Omega(g))$ scales as $-g^2 \log(g)$. In the 1D parabolic case, the shift follows a $-g^{4/3}$ dependence. Finally, for the 2D chequerboard case, the shift exhibits the more complex scaling of $-g^{4/3} \log^{2/3}(g)$, highlighting the enhanced hybridization due to the higher-order Van Hove singularity in the JDOS.

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2.16 Phenomenology of a Rydberg impurity in an ideal Bose-Einstein condensate

AILEEN A. T. DURST, T. A. YOĞURT, AND MATTHEW T. EILES

Rydberg atoms primarily interact with their environment via electron scattering, making the electronic wave function the key determinant of the resulting interaction potential. When a Rydberg atom is immersed in a Bose-Einstein condensate (BEC), the composite system forms a quantum impurity problem amenable to a quasiparticle description. The many-body response reveals the formation of polarons and molarons – Rydberg atoms and molecules, respectively, dressed by the collective modes of the bosonic environment.

These are well-defined quasiparticles, appearing as sharp asymmetrical peaks in the absorption spectrum, when the average interparticle spacing $\rho^{-1/3}$ in the condensate is larger than or comparable to the s-wave scattering length of the Rydberg interaction a. In the opposite limit, the spectral response tends towards a Gaussian profile without any identifiable substructure. These same phenomenological limits are also identified in short-ranged (contact) polarons, ionic polarons, and Rydberg polarons with anisotropic interactions. This provides a physical link between the density shift well-known from pressure broadening and the many-body impurity response in the strongly interacting regime, and shows that these different impurities share the same underlying physics determined by the universal dimensionless parameter $a\rho^{-1/3}$.

Theory: The dynamics of strongly-interacting quantum mixtures pose a significant challenge to theoretical description, even at the level of a single impurity immersed in a non-interacting bath. In the co-moving frame of the Rydberg impurity, the many-body Hamiltonian is

$$\hat{H} = \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2\mu} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{q}} V(\mathbf{q}) \hat{b}^\dagger_{\mathbf{k}+\mathbf{q}} \hat{b}_{\mathbf{k}}, \tag{1}$$

where $\hat{b}^\dagger_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}$ denote the bath creation and annihilation operators, $V(\mathbf{q})$ is the interspecies interaction, and μ is the impurity-boson reduced mass. Rydberg atoms interact with ground-state atoms via a short-range potential proportional to the electron-atom scattering length a_s. After integrating out the electronic motion and applying a magnetic field to lift the possible degeneracy of the electronic Rydberg states and impose a lab-frame orientation, the two-body interaction potential directly mirrors the electronic wave function itself:

$$V(\mathbf{R}) = 2\pi a_s \left|\phi_{nl}(R)\right|^2 \left|Y_{lm}(\hat{R})\right|^2. \tag{2}$$

Here, nlm are the principal and angular momentum quantum numbers describing the electronic state, and $\phi_{nl}(R)$ and $Y_{lm}(\hat{R})$ are the radial and spherical components of the Rydberg wave function. This interaction is generally long-ranged and oscillatory; additionally, for non-zero l it is anisotropic.

To investigate and characterize the universal aspects of the Rydberg impurity, we performed a detailed numerical study of the absorption spectrum $A(\omega)$. This is obtained from the Fourier transform of the autocorrelation function

$$S(t) = \langle e^{i\hat{H}_0 t} e^{-i\hat{H}t} \rangle = \left(\sum_\alpha e^{i(\epsilon_0 - \omega_\alpha)t} \left|\langle 0|\alpha\rangle\right|^2 \right)^N, \tag{3}$$

where the expectation value is taken with respect to the non-interacting BEC state (the ground state of $\hat{H}_0$) and N is the number of bosons. The final expression of the many-body response only requires the eigenstates ($|0\rangle$), $|\alpha\rangle$ and energies (ϵ_0), ω_α of the (non)-interacting two-body Hamiltonian of the Rydberg atom and a single boson. Allowing for the possibility of anisotropic interaction potentials, we expand the two-body wave function into spherical harmonics, $\langle \mathbf{R}|\alpha\rangle = \sum_{L,M} \chi^\alpha_{LM}(R) Y_{LM}(\hat{R})\, Y_{LM}(\theta_R, \phi_R)$, to obtain the coupled radial Schrödinger equations

$$\begin{aligned} 0 = &\left(-\frac{\nabla^2_R}{2\mu} + \frac{L(L+1)}{2\mu R^2} - \omega_\alpha \right) \chi^\alpha_{LM}(R) \\ &+ \sum_{L',M'} 2\pi a_s \left|\phi_{nl}(R)\right|^2 \chi^\alpha_{L'M'}(R) \langle LM|Y^*_{lm} Y_{lm}|L'M'\rangle. \end{aligned} \tag{4}$$

The off-diagonal terms in Eq. 4 include inelastic scattering processes in which bath particles scatter from one angular momentum state to another.

Results: Exemplary absorption spectra are shown in Fig. 1. Panels (a) and (b) illustrate the case of spherically symmetric and anisotropic interactions, respectively. In both cases, polaron formation is signaled by the displacement of the bare atomic peak from zero energy and its asymmetric profile [1]. As long as $a\rho^{1/3}$ is sufficiently small, the polaron's energy shift is characterized by the mean-field energy $E_{\mathrm{Pol}} = 2\pi\rho a/\mu$ (green curve in Fig. 1(a)) for a spherically symmetric potential. For anisotropic potentials, where the scattering continuum is necessarily multichannel, we instead have to consider the energy-analytic K^0-matrix [2] instead of the single channel quantity a. In the zero energy limit, only the s-wave component of the K^0 matrix, K^0_{00}, is non-zero, and we set $a \equiv K^0_{00}$ for an anisotropic potential (see Fig. 1(b)) [3].

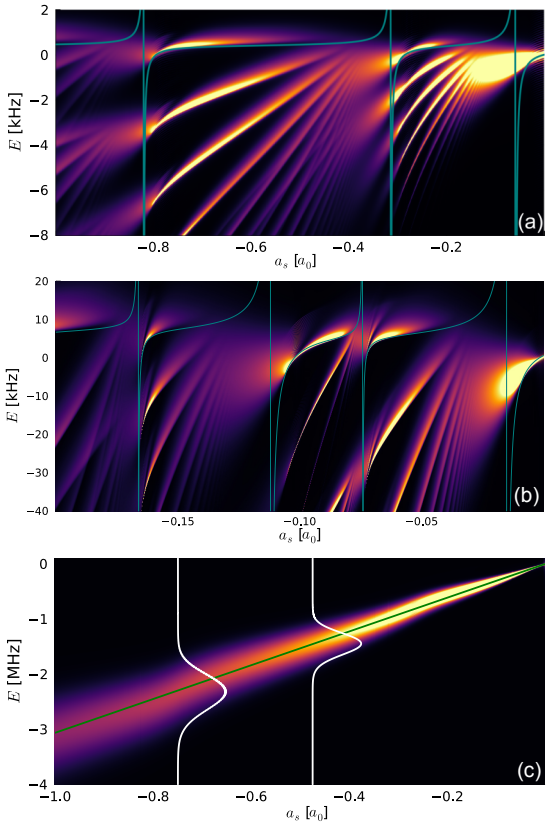

Figure 1: The absorption spectrum $A(\omega)$ of three different Rydberg impurities. The Rydberg state and BEC density are: (a) $50S$, $\rho = 10^{12}\,\mathrm{cm}^{-3}$; (b) $25P$, $\rho = 7\times10^{14}\,\mathrm{cm}^{-3}$, and (c) $50S$, $\rho = 1\times10^{14}\,\mathrm{cm}^{-3}$. In (a) and (b), E_{Pol} is shown in the green curve. In (c) cuts at fixed a_s (white curves) show the lineshape and the density shift E_{Ryd} is shown in green.

As the two-body potential deepens, it supports multiple bound states which manifest as "molarons" in the absorption spectrum. These are polyatomic molecules which, in the same way as the bare Rydberg atom, are dressed by the surrounding gas via the long-range Rydberg-atom interaction. For the anisotropic potential, particles in the $L = 0$ channel can tunnel through the centrifugal barrier of the $L > 0$ scattering channels to occupy these bound states, manifesting as Feshbach resonances.

As the density increases, $a\rho^{-1/3} \gg 1$, and a macroscopic number of bosons accumulate inside the Rydberg atom. The details of the molecular states vanish and melt into a continuum of many-body states with a Gaussian envelope, (Fig. 1(c)). The mean value of this envelope is given by the density shift $E_{\mathrm{Ryd}} = \rho\int \mathrm{d}^3 r V(\mathbf{r}) = 2\pi a_s\rho$. This density shift is independent of the Rydberg state, highlighting its fundamental nature. Remarkably, this universal feature —characterized by zero quasiparticle weight— emerges also in the unitary regime $a \to \infty$ as well, revealing the connection between an impurity in a high density regime and one in a strongly interacting regime [1, 3]. This same universal behavior is seen also for other types of impurities [1].

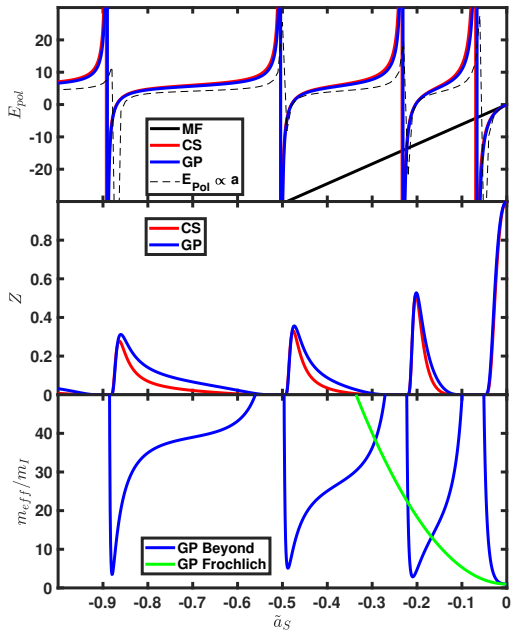

Figure 2: Quasiparticle properties of a Rydberg impurity in a weakly interacting Bose condensate ($a_{BB} = 100a_0$, $\rho = 10^{13}\mathrm{cm}^{-3}$), calculated by the coherent state ansatz (red) and the perturbative Gross-Pitaevskii theory (blue): (a) The polaron energy E_{pol}, (b) the quasiparticle weight $Z = S(t\to\infty)$, and (c) the effective mass m_{eff}. The dashed line in (a) shows E_{Pol} and the solid black line is E_{Ryd}.

Outlook: To better understand the nature of these quasiparticles, we are developing additional numerical methods: the coherent state ansatz, which treats the impurity-bath problem through the coherent excitations of the phonons within the condensate, and the perturbative Gross-Pitaevskii theory, which calculates the perturbations over the uniform condensate density due to the presence of a moving impurity [4]. Despite their distinct formulations, both approaches exhibit a strong qualitative agreement in capturing the quasiparticle properties of a Rydberg impurity (see Fig. 2). The presence of relatively finite quasiparticle weights Z between the resonances shows, in agreement with our previous work, that the Rydberg impurity sustains a quasiparticle character when $a\rho^{1/3} \ll 1$. However, for higher condensate densities, Z approaches arbitrarily small values, thereby reducing the validity of the polaron description for the Rydberg impurity and calling into question the interpretation of prior experimental observations [5].

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2.17 Precision spectroscopy and non-adiabatic stabilization of Rydberg molecules

FREDERIC HUMMEL, AILEEN A. T. DURST, MILENA SIMIĆ, AND MATTHEW T. EILES

Recent efforts to understand and harness ultracold molecules including both Rydberg and ground-state atoms among their constituents have become increasingly sophisticated. The expansion of experimental platforms to incorporate optical tweezer arrays, dual species traps, ion microscopes, and high-resolution momentum spectroscopy in their exploration of these exotic molecules has motivated the development of new theoretical treatments to reach spectroscopic accuracy in their description of long-range Rydberg molecular structure. We have formulated a method based on the Coulomb Green's function to obtain highly accurate adiabatic potential energy curves and vibrational spectra, and investigated the effects of vibronic coupling induced by non-adiabatic physics. Employing both of these developments, we predicted and, in an joint experiment-theory collaboration, observed a striking consequence of the breakdown of the Born-Oppenheimer approximation.

A long-range Rydberg molecule (LRRM) is an electronically excited bound state of a Rydberg atom and a ground-state atom. An accurate understanding of these unusual molecules is important for the study of impurity dynamics in ultracold gases, the design of quantum information retrieval protocols, precision measurements of electron-atom collisions, and the wider study of ultracold chemistry. The Born-Oppenheimer potential energy curves (PECs) describing the structure of LRRMs are determined by the eigenenergies of the electronic Hamiltonian $\hat{H}$ parametrically dependent on the internuclear distance R. This Hamiltonian incorporates the fine and hyperfine structure of both atoms and up to six electron-atom scattering channels to describe the electron-atom interaction using an extended Fermi pseudopotential.

The standard method used to obtain molecular PECs for LRRMs, involving the expansion of $\hat{H}$ into a basis of atomic Rydberg states, suffers from several flaws that make it unsuitable for precision calculations. Most significantly, this expansion is known to not converge because of the pseudopotentials utilized. We have developed a novel method employing the Coulomb Green's function to compute the PECs in terms of the roots of an analytical determinantal equation [1]. This treatment circumvents any difficulties related to the basis expansion's convergence and significantly improves on its precursors, which did not include the relevant spin degrees of freedom and relativistic effects.

Fig. 1 shows exemplary PECs descending from the dissociation threshold of the ^{87}Rb $27F_{7/2}$ atomic level. Three PECs possess potential wells deep enough to support vibrational states; the two drawn in black are experimentally accessible from spin-polarized atoms in the $f = 1$ hyperfine state and correspond to the polar "trilobite" electronic states. Several PECs corresponding to "butterfly" electronic states plummet steeply down due to the p-wave shape resonance present in Rb. They destabilize the trilobite PECs, removing any inner barrier in the adiabatic PECs above -6 GHz. The inset shows the vibrational spectrum of trilobite states measured by our collaborators at RPTU Kaiserslautern-Landau via three-photon photoassociation spectroscopy [2]. The measured and calculated binding energies agree to better than 1%, an accuracy only achievable because of our improved calculation; the PECs produced using the basis expansion method (displayed in dashed blue) possess uncertainties of up to 10% due to their poor convergence. No higher lying vibrational states are observed, consistent with the disruption caused by the p-wave resonance.

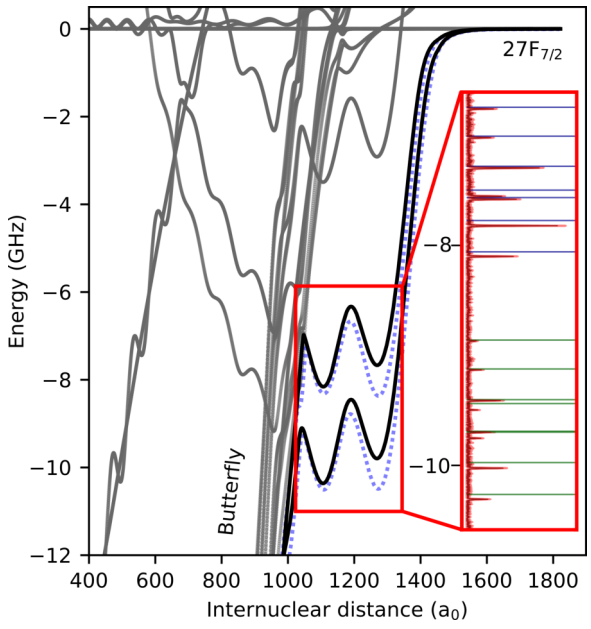

Figure 1: Born-Oppenheimer potential energy curves (PECs) below the $27F_{7/2}$ dissociation threshold obtained using the Green's function treatment (grey,black) and basis expansion (dashed blue). Vibrational levels bound in the black PECs are experimentally accessible. The inset shows the measured vibrational spectrum (red) and the calculated binding energies in the lower (green lines) and upper (blue lines) PEC [2].

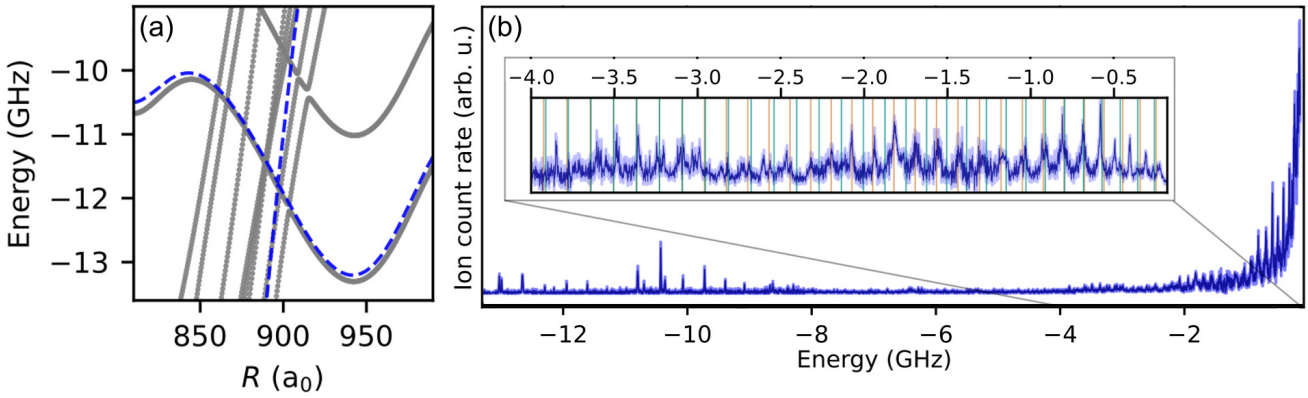

Figure 2: (a) Trilobite PECs computed using the Green's function treatment (gray) and the two-state model (blue). (b) Vibrational spectrum (measured by counting ions after ionizing the LRRMs) as a function of the detuning from the ^{87}Rb $25F_{7/2}$ atomic state. The shaded area indicates the ion count rate error. The inset shows a magnification of the highly excited vibrational spectrum, using a linear scaling to improve the visibility. The overlaid stick spectrum shows the computed vibrational levels bound in the pure trilobite PECs [6].

A second potential source of error in our quantitative description is the Born Oppenheimer approximation, which is violated in the vicinity of narrow avoided crossings such as those seen scattered throughout the PEC landscape of Fig. 1. To this end, we have systematically explored non-adiabatic coupling in LRRMs [3–5]. Although significant numerical effort is necessary to quantitatively treat vibronic coupling and account for predissociation and multichannel effects [3, 4], a surprising amount of insight into the overall behavior of the non-adiabatic processes can be gleaned from effective models [5]. As a particularly intriguing example, we found that the strength of the avoided crossing between the "trilobite" and "butterfly" PECs, which depends sensitively on the principal quantum number n, is predicted via a two-state model [5]. From this model, we obtained the equations

$$u_{n0}(R) = 0 \text{ and } (R/2n^2)^{-1} = (1 + (k_{SP}n)^2)^{-1} \quad (1)$$

that, when simultaneously satisfied as a function of n and R, allow the avoided crossing to close. Here, $u_{n0}(R)$ is the S-state radial wave function of the hydrogen atom and $k_{SP}^2/2 \approx 8.37$ meV is the energy where the s and p-wave $e-$Rb scattering phase shifts are identical. Eq. 1 has (among others) solutions at non-integer $n = 25.216$ and $n = 28.978$, implying that LRRMs associated with the nearby *integer-valued* $n = 25$ and $n = 29$ will exhibit very narrow avoided crossings.

As seen in Fig. 2(a), the $n = 25$ PECs indeed exhibit extremely narrow avoided crossings. The Landau Zener crossing probability P_{LZ} effectively characterizes the influence of the avoided crossing on non-adiabatic dynamic P_{LZ} is in excess of 99% for $n = 25$, while it is less than 60% for $n = 27$. This implies that vibrational states in the former case do not experience the destabilizing effect of the butterfly interaction as they hop from one Born-Oppenheimer surface to the other; the high-lying vibrational states utterly absent in the $n = 27$ spectrum should therefore be detectable for $n = 25$.

Fig. 2(b) shows the complete vibrational spectrum of a $n = 25$ trilobite molecule [6]. In accordance with the above prediction, a vibrational series close to the dissociation threshold is clearly seen. Upwards of thirty peaks with a spacing of ~ 120 MHz are observed, and we assigned vibrational quantum numbers $\nu \sim 70-100$ to these levels by comparison with the theoretical spectrum of the pure (diabatic) trilobite PECs. The calculated (stick spectrum) and observed series shown in the inset of Fig. 2(b) are in very good agreement. The dearth of vibrational states at intermediate detunings is a consequence of their negligible Franck-Condon overlaps [6].

In conclusion, we have improved the theoretical description of LRRMs, enabling the calculation of their vibrational spectra to an unprecedented precision and motivating the study of analytically tractable models yielding sharp physical insight. This led to the prediction and subsequent observation of highly excited vibrational states of LRRMs stabilized by non-adiabatic coupling. The Green's function treatment also proved instrumental in the theoretical assignment of vibrational spectra for Rb-Cs LRRMs assembled from atoms trapped in optical tweezers [7] in collaboration with the Cornish lab at Durham University, confirming its utility across different atomic species, Rydberg levels, and experimental setups.

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2.18 Random Yielding Transition and Emergent Chirality in Cell Spheres

MARKO POPOVIĆ AND FRANK JÜLICHER

Cell spheres A key problem in Biology is to understand how the collective organization of many cells emerges from the interplay of active cellular processes and cell interactions. An important model system are cell spheres, which can undergo complex remodeling and even morphogenesis, and which form the basis of organoid systems. We have studied the collective dynamics of cells in pancreas spheres as a simple model system of cellular self-organization. Pancreas spheres are embedded in a gel-like matrix. They often exhibit spontaneous rotations as a result of collective cell migration on the matrix [1] (see Figure 1). During these rotations, cells move relative to the matrix and can coordinate their motion via mechanical or chemical interactions. We can observe cell movements in three dimensions and represent cell dynamics by projecting velocities on the surface of a sphere. This quantification reveals cell flows, cell rearrangements and also cell shape changes leading to an emergent overall rotation of the cell sphere.

Vertex model on a sphere In order to investigate the principles of self-organization of the cell dynamics on the sphere, we use a vertex model that captures key features of cell mechanics and emergent collective cell motion of the surface of a sphere [1, 2]. Cells are represented by polygons with vertices confined to a sphere, see Figure 2. A work function

$$W = \sum_{\alpha \in \text{cells}} \left[\frac{1}{2} K (A_\alpha - A^{(0)})^2 + \Lambda L_\alpha \right] \qquad (1)$$

describes tissue forces via the infinitesimal work associated with vertex displacements. The dynamics of vertex positions $\mathbf{X_m}$ is determined from the balance of vertex forces $\mathbf{f}_m = \partial W / \partial \mathbf{X}_m$ and cell traction forces at vertex m as

$$\xi \dot{\mathbf{X}}_m = F \langle \mathbf{p} \rangle_m - \frac{\partial W}{\partial \mathbf{X}_m} + \hat{f}_m \hat{\mathbf{n}}_m \quad . \qquad (2)$$

Here $\dot{\mathbf{X}}_m$ denotes the vertex velocity and ξ is a friction coefficient describing friction of cells with respect to the matrix. The active part of the traction force stems from cellular force generation with magniutude F in the direction of the cell polarity unit vector $\mathbf{p}$. At a vertex m, this force is governed by the net polarity $\langle \mathbf{p} \rangle_m = \sum_{(\alpha|m)} \mathbf{p}_\alpha / M_\alpha$, of cells α that are adjacent to vertex m, where M_α denotes the number of vertices of cell α. Finally, $\hat{f}_m$ is the magnitude of the force in direction of the surface normal $\hat{\mathbf{n}}_m$ that constrains vertices to the sphere surface.

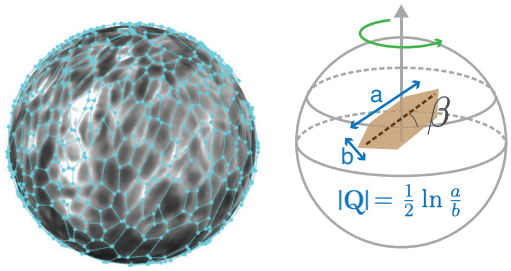

Figure 1: Pancreas sphere organoid. The shape of cells is segmented (left, blue lines) and quantified by a nematic tensor $\mathbf{Q}$. The sphere exhibits spontaneous rotation and emergent chirality. The chirality is revealed in asymmetric orientation of the cell elongation nematic described by the angle β with respect to the lines of latitude (right).

The time evolution of the polarity $\mathbf{p}_\alpha$ of cell α follows the dynamics

$$\frac{D\mathbf{p}_\alpha}{Dt} = \gamma \langle \mathbf{p}_\alpha \rangle + \sqrt{2D_r}\eta(t) + \mu \mathbf{p}_\alpha + p_\alpha^n \hat{\mathbf{n}}_\alpha \quad . \qquad (3)$$

Here D/Dt denotes a corotational derivative taking into account net polygon rotation of cell α. The coefficient γ describes the rate of polarity alignment of cell α to the average of its neighbors $\langle \mathbf{p}_\alpha \rangle$. Noise is introduced by the rotational diffusion coefficient D_r and μ is a Lagrange multiplier to maintain $|\mathbf{p}_\alpha| = 1$. Finally the contribution p_α^n ensures that the polarity vector remains tangential to the sphere surface.

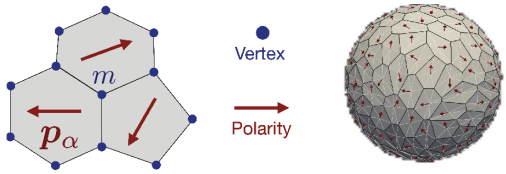

Figure 2: Vertex model on a sphere. Cells are described by polygons with vertices lying on the surface of the sphere. Each polygon is associated with a polarity vector $\mathbf{p}$, characterizing structural polarity of the cell (left). An example of a configuration with disordered polarity is shown (right).

In the absence of active traction $F = 0$ and low noise, the system is solid and cells do not move. Polarity organizes in a pattern with two $+1$ topological defects. As active traction is increased, the solid state will rotate because the polarity pattern generically has broken chiral symmetry and spirals towards the defects. The overall rotation pseudo-vector $\mathbf{\Omega}$ follows from the fact that the net external torque must vanish. The resulting motion is rather regular rotations of a solid cell packing. At a critical value of the active traction F, a yielding transition occurs, which is a dynamic phase transition [2]. Traction forces become strong enough to induce cell rearangements and cause cell flows. Beyond

this yielding transion, the system generates cell flows on the sphere and the polarity changes dynamically and loses larger scale order. Therfore in this regime rotations become irregular with fluctuating rotation axis or even leading to random cell movements without discernible rotations. These behaviors are summaried in the state diagram shown in Figure 4. Near the yielding transition, the system may stochastically transition between transient phases of regular solid rotation irregular flow behaviors.

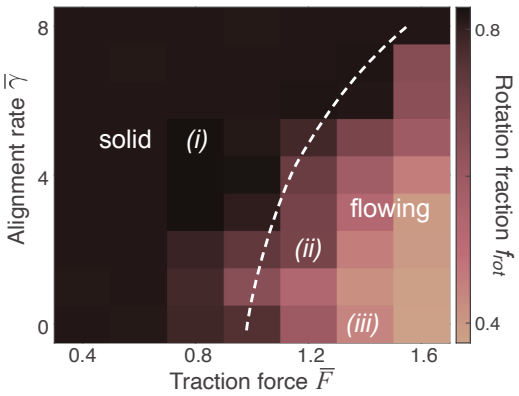

Figure 3: Dynamic phase diagram of solid to flowing transition. The alignment rate γ describes the neighbor coupling of cell polarity, the traction force amplitude F drives flows and cell rearrangements. The rotation fraction, i.e. the contribution of rigid body rotation to collective cell motion is shown as color code. In the solid regime (i), rigid rotation occurs, after the flow transition (ii) rotating motion becomes irregular in the flowing regime (iii).

Emergent Chirality of pancreas spheres The observed cell dynamics and rotations of pancreas spheres can be explained using our theoretical results. The rotatory motion reveals an underlying cell polarity pattern on a sphere that exhibits chiral asymmetry, resulting in a net rotation. The different regimes observed, with some spheres showing regular rotations over long times, while others intermitttent and more irregular behaviors, suggests that pancreaes spheres operate in the viscinity of the yielding transition [1].

The broken chiral symmetry is not revealed by the rotation alone. A rotating sphere is characterized by a single pseudovector $\mathbf{\Omega}$ but is otherwise rotation invariant. Therefore it is invariant with respect to an inversion in space, followed by a rotation by 180°, which maps $\mathbf{\Omega}$ to $-\mathbf{\Omega}$, and therefore is not chiral. However, when observing patterns of cell shape on the sphere surface, the chirality of the sphere becomes evident. Cells are typically slightly elongated. This elongation defines a cell nematic that characterizes cell shape. Analysis of cell packings reveals that the angle β of the cell elongation axis with respect to the azimuth is typically oriented either 45° or 135° with respect to the azimuth, when the rotation vector $\mathbf{\Omega}$ points along the z axis, see Figure 1. This configuration is chiral because it is not invariant with respect to any transformation that involves an inversion of space.

This emergent chirality is a consequence of the underlying chirality of the polarity field that generates the rotations. In the vertex model this chirality is not emerging in the solid phase, in the absence of cell rearrangements. Cell rearrangements due to yielding or noise lead to cell flows that reveal the broken symmetry in the cell elongation patterns [1]. The emergence of chirality in the cell morphology can be discussed using a continuum theory on the sphere. The polarity then satisfied the dynamic equation

$$\partial_t \mathbf{p} + \mathbf{v} \cdot \nabla \mathbf{p} - \omega \times \mathbf{p} = \Gamma \nabla^2 \mathbf{p} \tag{4}$$

where ω denotes the vorticity of the surface flow $\mathbf{v}$. The surface flow is obtained from the balance of traction forces and material stresses on the surface $\nabla \cdot \sigma = F\mathbf{p} - \xi\mathbf{p}$, where σ denotes the tangential stress tensor on the surface.

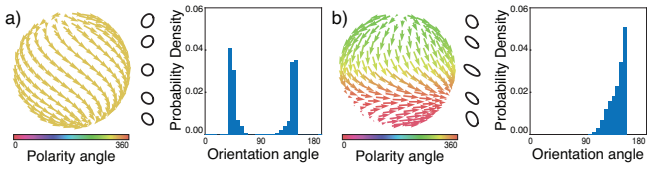

Figure 4: Polarity patterns on a sphere. (a) Polarity patterns in the solid state without flows. The distribution of the cell elongation angle β is symmetric and does not reveal chirality. (b) In the presence of flows the symmetry of the polarity pattern is broken and chirality emerges in the distribution of cell elongation angles. The ellipses indicate cell elongation patterns.

Discussion Organoids are simple model systems to study cellular self-organization in the context of morphogenesis. We have shown that pancreas spheres exhibit emergent chirality as a collective phenomenon. Cells on a sphere can undergo a self-driven yielding transition via active traction forces. This demonstrates the richness of active behaviors and material properties of cellular assemblies. Based on our work we will investigate in the future the role of tissue hydraulics in the formation of fluid filled lumina as a first step in the formation of networks of transport channels of the pancreas.

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2.19 Droplet Differentiation by a Chemical Switch

TYLER S. HARMON AND FRANK JÜLICHER

Biomolecular Condensates as organizers of biochemistry. Cells organize biochemistry in space through the formation of distinct chemical compartments. Compartments are often separated by a membrane from their environment, but many compartments do not have a membrane. Membraneless compartments are often dynamic assemblies of proteins and nucleic acids called biomolecular condensates. These condensates can protect molecules or may enable specific biochemical reactions. Therefore, biological condensates can organize biochemistry in space by providing reaction centers for particular biochemical processes or by positionig specific molecules in the cell. Liquid condensates are dynamic, molecules can diffuse inside to react, or to exchange quickly with the surroundings.

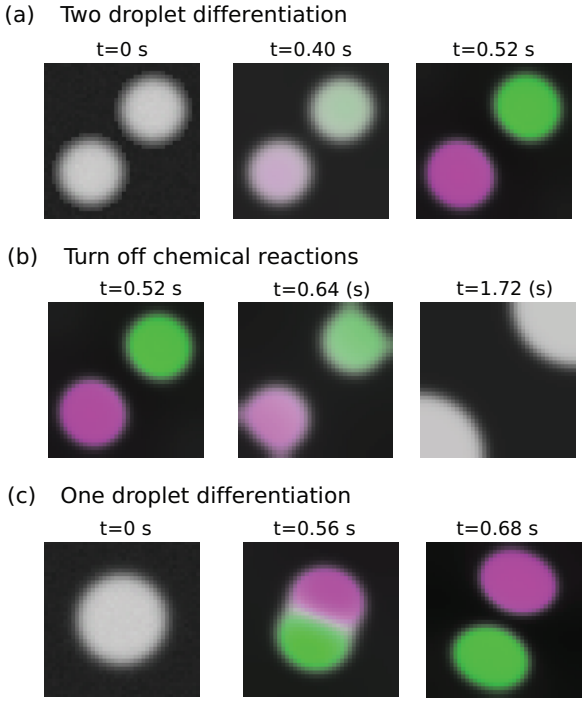

Figure 1: Differentiating droplets. (a) Two droplets initially containing equal amounts of A and B differentiate in an A-rich and a B-rich droplet. (b) As reactions are turned off, the system relaxes back to the initial state. (c) A single droplet demixes in A and B-rich domains which thens split and form two droplets.

Over the last decade, many different condensates have been identified. Examples are stress granules, P-granules or the nucleolus inside the cell nucleus. Different types of condensates have distinct characteristics and assemble specific molecules in a small compartment. A fundamental question in biology is to understand how distinct types of condensates can form in a cell to coexist, and what determines their identity. Condensates are best understood as a coexistence of liquid phases and thus as liquid droplets immersed in the cytoplasm. In a multicomponent system at equilibrium, several different phases can coexist according to the Gibbs phase rule. However the coexistence of many different types of condensates by multi-phase coexistence in the cell would require a fine tuning of parameters such that the mixture can be maintained in such a multi-phase coexistence regime.

Cellular biochemistry has different ways to modify molecules for example by phosphorylation or by ubiquitination. This requires enzymes that catalyze such modification reactions. Motivated by the idea that specific types of condensates could assemble by protein modification, we have investigated how a system of proteins and modification enzymes could together generate distinct condensate identities by an out-of-equilibrium differentiation process. This is explored in a system, which, in the absence of enzymatic activity, undergoes thermodynamic phase separation in two coexisting phases.

Simple model for droplet differentiation. We consider a simple model where a molecular component called scaffold phase separates from solvent S in a two-phase coexistence. The scaffold molecule can exist in two different forms, denoted A and B. Both A and B have very similar physical properties and therfore undergo phase separation together to form a dense phase that phase separates from solvent S. The component A can be modified to become B by an enzyme denoted AB, which consumes a fuel to drive this reaction forward. Similarly, the enzyme BA mediates the reverse modification of B to A in an active process. The phase separation can be described by the free energy

$$F = \int dV \left[f(n_i) + \frac{\kappa}{2} (\nabla n_S)^2 \right] \tag{1}$$

where we write the free energy density as

$$\begin{aligned} \frac{f}{k_B T} &= -\chi v (n_A + n_B + n_{AB} + n_{BA})^2 \\ &- \epsilon v (n_A - n_B)(n_{BA} - n_{AB}) + \sum_i n_i \ln n_i v \quad . \end{aligned} \tag{2}$$

Here, v denotes a molecular volume. The parameter χ describes interactions that favor phase separation of all components from solvent. The parameter ϵ describes an affinity of enzymes such that they tend to colocalize with their own reaction products, thus distinguishing A and B components. We describe the dynamics of all

concentrations by Cahn Hilliard equations, taking into account enzyme reactions

$$\partial_t n_A = \Gamma \nabla^2 \mu_A + r \tag{3}$$
$$\partial_t n_B = \Gamma \nabla^2 \mu_A - r \quad , \tag{4}$$

where

$$r = -k_{AB} \frac{n_{AB} n_A}{K_{AB} + n_A} + k_{BA} \frac{n_{BA} n_B}{K_{BA} + n_B} \quad , \tag{5}$$

is the reaction flux, and we have $\partial_t n_{AB} = \Gamma \nabla^2 \mu_{AB}$ and $\partial_t n_{BA} = \Gamma \nabla^2 \mu_{BA}$. Here, $\mu_i = \delta F / \delta n_i$ are the chemical potentials. Examples of droplet dynamics are shown in Figure 1. Droplet differentiation can occur for sufficiently strong chemical driving.

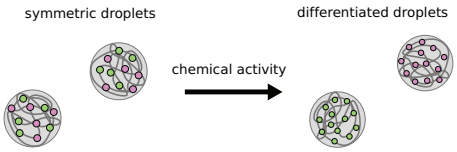

Figure 2: Schematic representation of droplet differentiation. Molecules A (red) and B (green) phase separate together from a solvent in a dense phase (grey). Enzymatic activity drives the system in a differentiated state where two droplets have different identity.

An enzymatic switch differentiates droplets. We now discuss the steady state droplets and their composition. The total scaffold and enzyme concentrations

$$n_s = n_A + n_B \quad , \quad n_e = n_{AB} + n_{BA} \tag{6}$$

are conserved and their total amounts remain fixed. As order parameters for droplet differentiation, we introduce the normalized concentration differences of scaffold and enzyme

$$\delta_s = \frac{n_A - n_B}{n_s} \quad , \quad \delta_e = \frac{n_{AB} - n_{BA}}{n_e} \quad . \tag{7}$$

We consider two droplets, both containing A and B at equal amounts, such that $\delta_s^- = 0$, where $-$ and $+$ refer to inside and outside the droplet, respectively. These droplets can either be stable or they can become unstable and differentiate in two droplets of different composition, one A-rich and one B-rich, see Figure 2. For the simmple case $k = k_{AB} = k_{BA}$ and $K = K_{AB} = K_{BA}$, the two mixed droplets become unstable with respect to differentiation when $\epsilon v n_s^- > 2K/(2K + n_s^-)$ and k exceeds a critical value such that

$$k \left[\frac{2\epsilon v n_s^-}{2K + n_s^-} - \frac{4K}{(2K + n_s^-)^2} \right] > \frac{3 D_s^+ n_s^+}{R^2 n_s^- n_e^-} \quad , \tag{8}$$

where R denotes the droplet radius, see Figure 3. Interestingly, even a single droplet can become unstable and divide asymmetrically, by differentiating in two differen droplets, see Figure 1 (c).

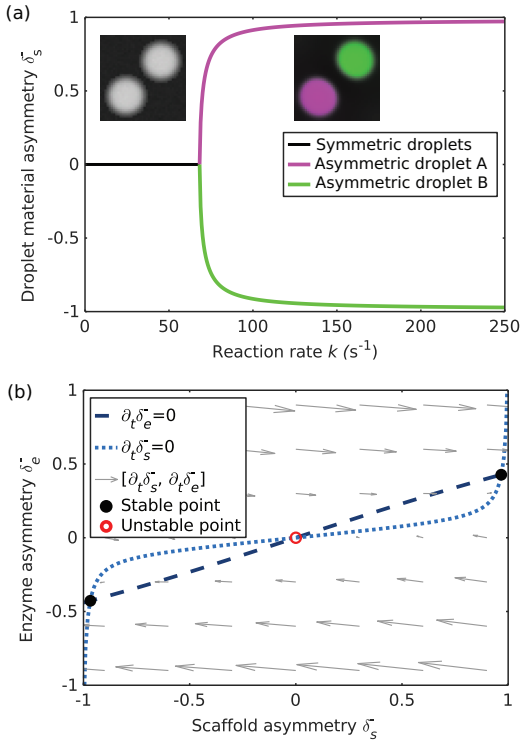

Figure 3: Droplet instability. (a) For small reaction rate k, symmetric droplets containing both A and B componet are stable (grey). Beyond a critical value of k, symmetric droplets are unstable and diferentiate in an A-rich (red) and a B-rich droplet via a pitchfork bifurcation. (b) Fixpoints and nullclines in the $\delta_s^- - \delta_e^-$ plane. Symmetric droplets correspond to an unstable fixpoint (red circle), differentiated droplets correspond to stable fixpoints (black circles). The dashed and dotted lines show nullclines and the grey arrows show the flow field describing the dynamics.

Active droplets as organizers of specific biochemistry. These results show different condensates with specific identities can emerge from simple 2-phase coexistence via enzymatic modifications of molecules, when enzymes operate out-of-equilibrium. This principle could account for the assembly of different condensate types in a cell using non-specific phase separation together with specific chemistry. The emergence of condensate identity and switches between droplet states shows that droplets can enable biochemical modules with complex functions. As an illustration for the versatility of droplets to enable surprising biochemical function, we have recently shown that molecular assembly lines can emerge via self-organization in droplets. Such systems permit the assembly of molecular complexes at low error rate in non-equilibrium conditions [2].

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2.20 Inference of Long-range Correlated Stochastic Models and Application to Predictions

JOHANNES KASSEL AND HOLGER KANTZ

Long-range correlations Edwin Hurst, a British hydrologist, discovered long-range temporal correlations (LRC) while estimating the optimal reservoir size for the river Nile in the 1950s. LRC are characterised by a slow decay of the autocorrelation function of a time series which leads to the divergence of its integral. This marks the absence of a characteristic time scale of the underlying process, a major difference compared to Markovian processes. LRC are typically satisfied by a power-law decay of the autocorrelation function determined by the Hurst exponent H, $C(\tau) \sim \tau^{2H-2}$, and $1/2 < H < 1$. Benoît Mandelbrot discovered that LRC also imply a fractal structure in time with a self-similarity determined by the Hurst exponent [1]. LRC imply persistent dynamics which lead to larger confidence intervals when estimating temporal averages and trends as well as clustered extremes.

The first empirical model possessing LRC was fractional Brownian motion, introduced by Benoît Mandelbrot and co-workers in 1968. It is a generalisation of Brownian motion, a Gaussian continuous-time stochastic process with mean zero and covariance function

$$C(t,s) = 1/2\,(|t|^{2H} + |s|^{2H} - |t-s|^{2H})\,. \qquad (1)$$

However, Mandelbrot's model did not gain popularity for some time due to its inability to model short-range behaviour and the consequential inaptness for geophysical application. Later on, both Hosking as well as Granger and Joyeaux independently introduced the auto-regressive fractionally integrated moving average (ARFIMA) process class, an extension of the popular discrete-time ARMA process class already well-known and established in the time series analysis and econometrics communities at that time. Its simplest non-trivial member, the ARFIMA(1,d,0) process, reads

$$x_{n+1} = \phi\, x_n + \sum_{j=0}^{\infty} \frac{\Gamma(d+j)}{\Gamma(d)\Gamma(j+1)}\, \xi_{n-j}\,, \qquad (2)$$

in which ϕ denotes the autoregressive parameter, $d = H - 1/2$ the memory parameter, $\Gamma(\cdot)$ the Gamma function and ξ Gaussian white noise with mean zero and variance one. For $\phi < 1$ and $0 < d < 1/2$, it models stationary over-damped LRC dynamics and due to the auto-regressive parameter may also describe short-range behaviour.

In the following, we present two methods for inferring nonlinear LRC stochastic models from single time series. Subsequently, we use the latter method to reconstruct stochastic models from temperature time series. We then use them for predictions and show that incorporating LRC in stochastic predictions improves the forecast horizon.

Inferring fractional diffusion equations The first reconstruction method maximises the path probability of a fractional stochastic differential equation (SDE) such that an observed trajectory becomes the most probable path [3]. We consider an over-damped stochastic differential equation with a deterministic, potentially nonlinear force $f(x)$, a diffusion term $g(x)$ that is space-dependent, driven by fractional Gaussian noise ξ^H with Hurst parameter H, the increment process of the fractional Brownian motion mentioned before, interpreted in the Ito sense.

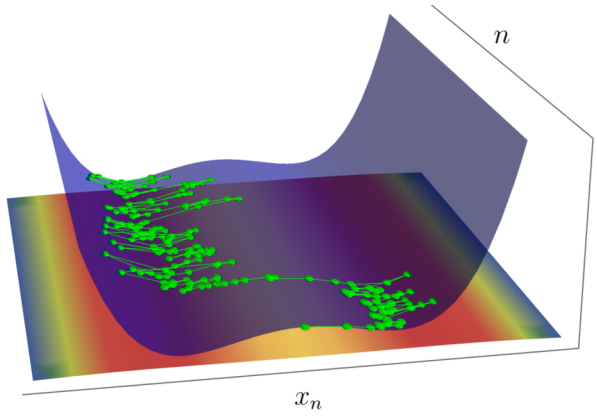

Figure 1: Sampled stochastic process in a double-well potential with multiplicative fractional noise. The noise magnitude is determined by the diffusion term, e.g. a temperature, illustrated by the colour of the bottom layer in the figure. Taken from [3].

We then derive a maximum likelihood estimator, which is given by

$$P \sim \exp(-\mathcal{S}[f,g|x]) \qquad (3)$$

with:

$$\mathcal{S} = -\frac{1}{2}\sum_{m,n=1}^{N} \frac{x_m - x_{m-1} - f(x_{m-1})\Delta t}{g(x_{m-1})} C^{-1}_{m,n} \frac{x_n - x_{n-1} - f(x_{n-1})\Delta t}{g(x_{n-1})} - \sum_{n=1}^{N} \ln|g(x_{n-1})|\,, \qquad (4)$$

which we interpret as a stochastic action. This estimator generalises the Onsager-Machlup theory of Markovian processes and is therefore named *fractional Onsager-Machlup optimisation* (fOMo). Maximising the likelihood is synonymous with minimising the stochastic action, which is a function of the parameters of drift f and diffusion g. In a synthetic data study, we show that neglecting LRC leads to large errors in reconstructed drift and diffusion functions even for Hurst exponents which deviate slightly from $H = 0.5$. We apply the method to daily mean temperature time series recorded at Potsdam Telegrafenberg weather station which possess $H = 0.65$, reconstructing an effective stochastic model that captures the statistics of the original time series well. The method is applicable for arbitrary correlation functions of Gaussian noises and allows for the inference of real physical parameters.

Inference via fractional differencing The second inference method reconstructs phenomenological stochastic models from time series and relies on the inverse relation of fractional differencing and integration [2]. We remove LRC from a time series by applying a fractional filtering operation which is the inverse of the fractional integration in ARFIMA processes:

$$x'_t = \lim_{M\to\infty} \sum_{n=0}^{M} \frac{\Gamma(j-d)}{\Gamma(j+1)\Gamma(-d)}\, x_{t-n}\,. \tag{5}$$

In real-world applications, the memory length M needs to be truncated. After performing the fractional differencing, we infer a Markovian over-damped stochastic difference equation of the form:

$$x'_{n+1} = f(x'_n) + g(x'_n)\,\xi_{n+1}\,, \tag{6}$$

in which ξ_n is Gaussian white noise with zero mean and variance one. The terms f and g act like drift and diffusion in the continuous-time Langevin equation, which we determine via maximum-likelihood estimation. Generating time series using the reconstructed Markovian stochastic difference equation and subsequent fractional integration, we can generate data possessing similar statistical properties as the original data.

Forecasting Temperature Extremes We use the second reconstruction method to obtain stochastic models of daily maximum and minimum temperatures which we utilise for temperature forecasts [5]. The fractional integration signifies a conditioning on the process' history. Literature suggests LRC and atmospheric pressure patterns as sources for increased predictability. By mutual information analysis we confirmed that the AO index, which characterises the main mode of pressure variablity over the north Atlantic ocean, is a useful input for temperature forecasts. Subsequently, we infer nonlinear long-range correlated stochastic models and several base-line models for both daily maximum and minimum temperature data recorded at Visby Flygplats, a Swedish weather station with a long, uninterrupted data record located in the region where the investigated influence of the atmospheric pressure pattern is maximal. We develop a scheme for stochastic forecasting, perform ensemble forecasts and take their mean as prediction. As one can see in Fig.2, the optimal model pushes the forecast limit significantly into the future.

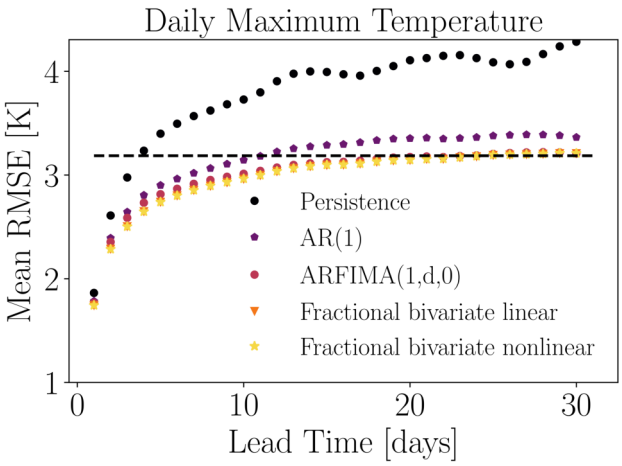

Figure 2: Forecast performance of various models as a function of the forecast lead time. The black dashed line indicates the standard deviation of the test set. When the root-mean square error of a forecast crosses the black dashed line it loses predictive power. Fractional models incorporating LRC show significantly enhanced forecast horizon compared to models without LRC. Taken from [5].

We have thus not only introduced two generally applicable methods for inferring nonlinear LRC stochastic models but also showed that LRC indeed is an additional source for predictability from which data driven forecasts can benefit in practice.

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2.21 Scale dependent error growth and optimal weather forecast models

HOLGER KANTZ

Atmospheric multi-scale motion The dynamics of Earth's atmosphere take place on a wide range of spatial and temporal scales. Planetary waves such as Rossby waves cover a whole latitude circle of about 30,000km, while dust devils are turbulent eddies in the range of cm. Associated with their spatial extensions are life times which behave in a similar way: Large scale structures are long lived, small scale structures are very short lived, see Fig.1. These life times can be re-interpreted as instability. After a given structure has decayed, it is hard to predict by which structure it will be replaced. If other words, it is plausible that a scale dependent Lyapunov exponent which measures the sensitivity to errors in the initial conditions on the corresponding scale would be much larger on small scales than on large scales.

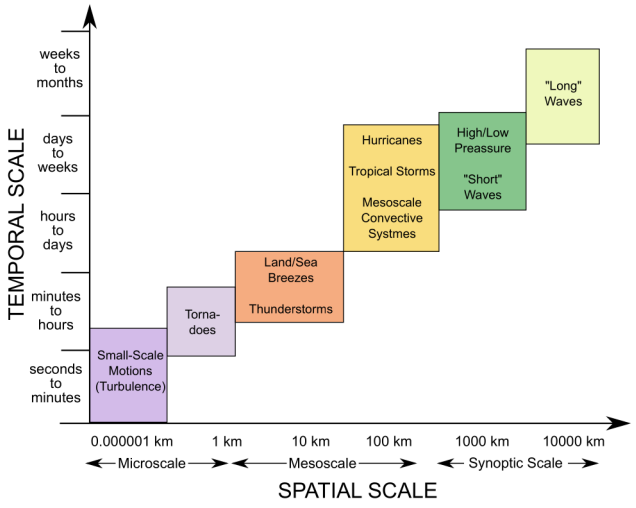

Figure 1: Spatio-temporal scales in atmospheric dynamics, taken from [2].

Such scale dependent error growth was indeed observed in certain model systems by a concept called 'finite size Lyapunov exponent' [1]. In [2] we introduced a hierarchical toy model which was inspired by the multi-scale properties of the atmosphere: We coupled identical dynamical systems, but rescaled in each both space and time such that the sub-system with the largest diameter of its chaotic attractor was also the slowest, i.e., its maximal Lyapunov exponent was small, and the sub-system with smallest diameter was the fastest. With this engineered system we could realise a scale dependent pseudo-Lyapunov exponent (not a proper Lyapunov exponent in the mathematically sense) which diverges on small scales like a power law, $\lambda(\epsilon) = a\epsilon^{-\beta}$ where the exponent β is determined by the spatial (α) and temporal (τ) scaling factors as $\beta = \ln\alpha/\ln\tau$. In this system, two initially nearby trajectories where one is assumed to carry an error E_0 in its initial condition will diverge from each other due to chaos, but since the divergence rate is dependent on the error magnitude and slows down for larger and larger errors, the error as a function of time grows like a power law in time: $E(t) = (E_0^\beta + a\beta t)^{1/\beta}$, see Fig.2. In the idealised case of infinitely many of such temporal and spatial scales, the true Lyapunov exponent is infinite. The striking consequence of this type of instability is the existence of a strictly finite prediction horizon even in the limit $E_0 \to 0$: $t_{\rm pred} = \frac{E_{\rm tol}^\beta - E_0^\beta}{a\beta}$, where $E_{\rm tol}$ is the maximally tolerable error for a useful forecast. This is a consequence of the property that the smaller the initial error is, the faster is its initial growth $\lambda(E_0) = aE_0^{-\beta}$.

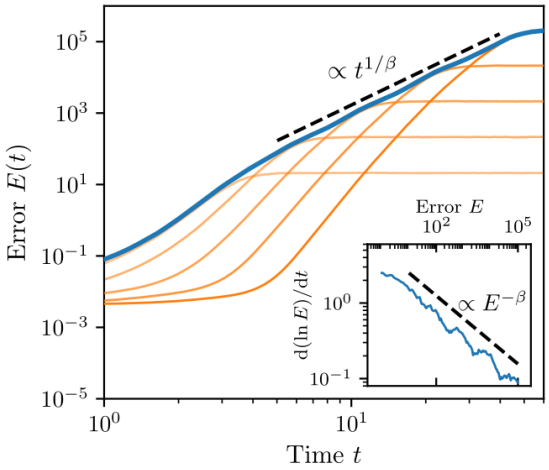

Figure 2: Power law error growth in the hierarchical toy model and the scale dependent Lyapunov exponent (inset). Orange lines show error growth in subspaces with saturation at smaller scales. From [2].

In [2] we re-analysed data of a numerical error growth experiment performed in [3] for an operational weather model: The authors of [3] followed pairs of initially very close trajectories and tracked how their distances grow as function of the already achieved distance. In a doubly-logarithmic representation we could show the compatibility of these data with the power law divergence of the Lyapunov exponent. Estimating the parameters a, β, E_0 we concluded that this very model had a strict upper bound for successful forecasts of 16 days, regardless of how accurate the true atmospheric state would be reconstructed.

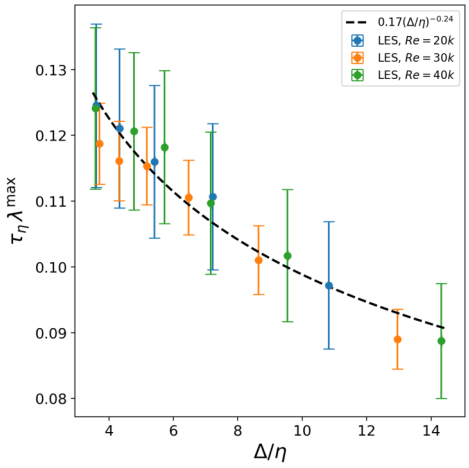

Figure 3: Maximal Lyapunov exponents in the model for turbulence diverge like an inverse power of the smallest resolved spatial scale Δ. Taken from [4].

Scale dependent error growth in turbulence A plausible explanation for the hypothesised scale dependent error growth in a weather forecast model is that this is a feature of turbulence. Therefore, together with the *distinguished PKS postdoctoral fellow* Burak N. Budanur, we studied a model for fully developed turbulence, namely the Kolmogorov flow. This is a periodically driven and sheared hydrodynamic flow in a cube with periodic boundary conditions, which, for suitable Reynolds numbers, exhibits turbulence. We compared direct numerical simulations DNS at hight spatial resolution to large eddy simulations LES, where the latter contain a given cut-off wave number. By reducing the cut-off wave number, LES simulation allowed us to include increasingly smaller scales. We could show numerically that the largest Lyapunov exponent of this system grows with the inverse of the cut-off wave number, Fig.3. This is therefore direct evidence of the claimed larger instability of motion on small scales compared to motion on larger spatial scales. The same simulations showed, as an additional result, a data collapse of the largest Lyapunov when spatial and temporal scales are measured in units of the Kolmogorov scale η and τ_η. For more details see [4].

Model error versus initial condition error in weather forecasting The second extension of previous work was done together with Hynek Bednář from the Department of Atmospheric Physics of the Charles University in Prague. A real weather forecast model contains the numerical implementation of the *primitive equations*. These are a set of coupled partial differential equations based on the principles of momentum conservation, continuity equation for mass, the conservation of energy, and the equation of state for the medium air. To be solved on a computer, the 3 dimensional continuum is discretised where the lattice spacing defines a lower cut-off for the spatial scales (state of the art: $\approx$ 20km for global models, $\approx$2km for regional models). For more accurate forecasts, weather agencies are reducing the lattice spacing for the inclusion of smaller scale processes in atmospheric dynamics. In view of the observed instability, there is an evident dilemma: Cutting off the small scales introduces model errors by ignoring relevant physics. Including the small scales, according to what we discussed before, the instability of model trajectories might be increased so that errors of the initial conditions would grow much faster as compared to a coarser model.

In our study [5] we analysed how the growth of these two types of errors, model errors versus initial condition errors, depend on the spatial resolution. Our focus was on how to maximise the forecast horizon, i.e., the number of days after which the forecast becomes useless because it has diverged too much from reality. Since a real weather forecast system cannot be operated by us, we chose the model for advection introduced by E.N. Lorenz in 1996 which mimics hydrodynamic transport due to westerly winds on a latitude circle of the globe. We extended it by introducing two levels of small scale motion which also have the properties to have larger Lyapunov exponents. First of all, we realised that model errors (i.e., the effect of the ignored small scale motion) causes a diffusive error growth: The fast degrees of freedom push the trajectory in a noise-like way, which is missing in the coarser model. Ignoring the 'noise', trajectories are smoother, but systematically wrong. The main conclusion of this work is that the model which resolves the small scale unstable motion is superior to the coarse grained model, however, the results are intricate and require further studies in the future. We therefore started an MSc project with Jennart Kuklinski which is devoted to a simpler setting where errors can be tracked more easily.

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2.22 Cell divisions imprint long lasting elastic strain fields in epithelial tissues

ALI TAHAEI AND MARKO POPOVIĆ

Epithelial tissues Epithelial tissues, or epithelia, are one of the four main types of biological tissues. They consist of tightly packed cellular sheets and in adult animals they cover body surfaces and line hollow organs. Epithelia also play an important role in animal development and participate in organ morphogenesis. For example, the wing of the fruit fly D. melanogaster, develops from a single epithelial layer of cells.

Understanding how mechanical forces affect epithelial tissues is a key challenge in animal development and regeneration. Biological tissues are often described as soft, viscoelastic materials that behave elastically over short timescales. However, over longer periods, they become more fluid due to processes such as cell divisions, extrusions, and intercalations, which gradually reshape the tissue.

When a cell in an epithelium divides, it generates deformation of the surrounding cells, potentially leading to cellular rearrangements and contributing to the overall tissue flow. Furthermore, divisions have been indicated to control the glassy cell dynamics in cultured epithelial tissues and embryonic tissues. However, despite the fact that cell divisions are a hallmark of biological matter, a quantitative understanding of the mechanical forces generated by cell divisions and their consequences are still lacking.

Cell divisions in the fruit fly wing epithelium We studied dynamics of dividing cells and the surrounding tissue in time-lapse movies of a growing fruit fly wing disc epithelium. At this stage, the wing disc epithelium consists of a single layer of cells whose apical surface was have imaged and analyzed over a period of about 13 hours [1]. An example of a cell division is shown in Fig. 1 A (i - iii). Notably, just before a division, the dividing cell increases its surface area. This is not due to cell growth, but rather due to three-dimensional reorganisation of the cell material preceding the division. Just after division, the two daughter cells have a joint surface area approximately equal to the area of their mother cell, as illustrated in Fig. 1 A (iv).

To characterize forces exerted by the dividing cell on the surrounding tissue we estimated the strain field $U_{ij}(\vec{r},t)$ in the tissue surrounding a dividing cell. For this, we measure changes of cell elongation tensor $Q_{ij}(\vec{r},t)$ and changes in cell areas $a(\vec{r},t)$, relative to the reference configuration defined at $t_0 = -60$ min before the division at $t_d = 0$ min. An example of the traceless-symmetric part of the shear strain $\tilde{U}_{ij} \simeq Q_{ij}(t) - Q_{ij}(t_0)$ is shown in Fig. 1 B (i - iii).

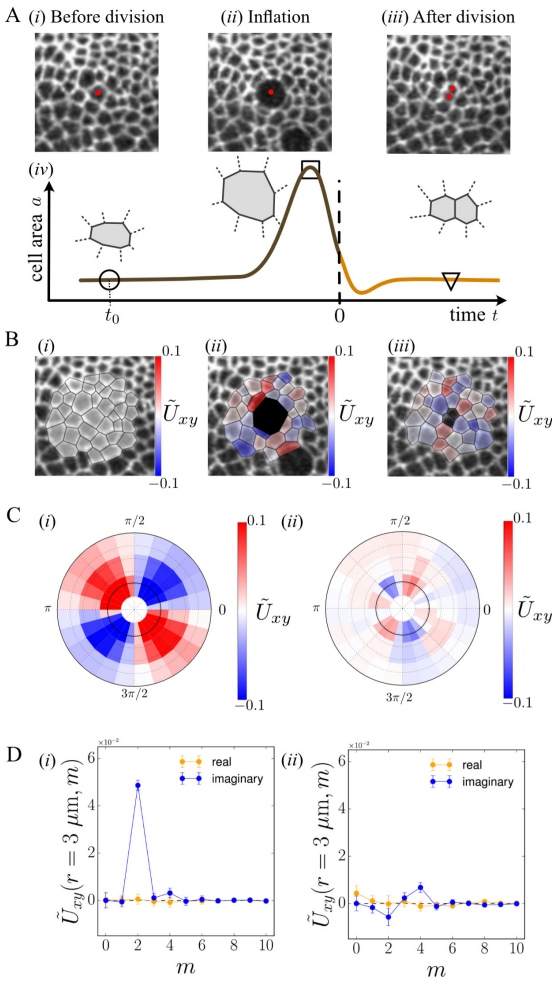

Figure 1: (A) Snapshots of a cell division in three stages. (A.*i*) As the mother cell (red dot) starts the division process, (A.*ii*) it rounds up, corresponding to area inflation, and then (A.*iii*) it shrinks and divides into the daughter cells (two red dots). (A.*iv*) A schematic representation of the cell area of the mother cell (brown) and the daughter cells (orange) during the division process. The symbols highlight the stage of the dividing cell before the division, at the peak of inflation, and after the division. The new bond forms at $t = 0$, and t_0 is the reference state. (B) Strain $\tilde{U}_{xy}$ of the cells near a typical cell division at the three stages shown in (A) with $t_0 = -60$ [min]. (C) Ensemble average ($N = 682$) of $\tilde{U}_{xy}$ around the dividing cell: (C.*i*) at the peak of the inflation $t = -20$ [min] (corresponding to (A.*ii*) and (B.*ii*)), and (C.*ii*) after the division $t = 30$ [min] (corresponding to (A.*iii*) and (B.*iii*)). The radial extent of the plots is $6\mu m$. (D) The angular Fourier transform of the $\tilde{U}_{xy}$ at a distance of $r = 3\ \mu m$ from the center of the mother cell at $t = -20$ [min] (D.*i*) and at $t = 30$ [min] (D.*ii*).

Averaging the strain field over an ensemble of cell divisions we identify relevant angular Fourier modes of the strain field: second and fourth modes for the traceless-symmetric strain (Fig. 1 C, D) and zeroth and second modes for the isotropic strain (Ref. [2]). Now, our aim is to infer the force distribution generated by cell division, from the observed strain pattern.

Cell division force dipole We propose to describe the fly wing epithelium as an elastic sheet, which allows us to predict the strain field generated by a localized force density field. Since the dividing cell is part of the tissue, during the division it cannot generate a net force on the surrounding cells, and the dominant force density component will be a force dipole. The force dipole tensor is represented by a symmetric matrix D_{ij}. Theory of linear elasticity provides an expression for the strain field

$$\begin{pmatrix} u_{kk}(\vec{r}) \\ \tilde{u}_{xx}(\vec{r}) \\ \tilde{u}_{xy}(\vec{r}) \end{pmatrix} = \frac{1}{2\pi K(1+\mu)} \mathbf{G}(\vec{r}) \begin{pmatrix} D_0 \\ \tilde{D}_{xx} \\ \tilde{D}_{xy} \end{pmatrix}, \qquad (1)$$

where u_{kk} is the isotropic strain, $\tilde{u}_{xx}$ and $\tilde{u}_{xy}$ constitute the traceless-symmetric strain, K is the shear elastic constant, μ is the ratio of shear to bulk elastic constants, and $G(\vec{r})$ is the elastic dipole propagator

$$\mathbf{G}(\vec{r}) = \frac{1}{r^2} \begin{pmatrix} \mathcal{N} & -\mu\cos 2\varphi & -\mu\sin 2\varphi \\ -\mu\cos 2\varphi & -\cos 4\varphi & -\sin 4\varphi \\ -\mu\sin 2\varphi & -\sin 4\varphi & \cos 4\varphi \end{pmatrix}. \qquad (2)$$

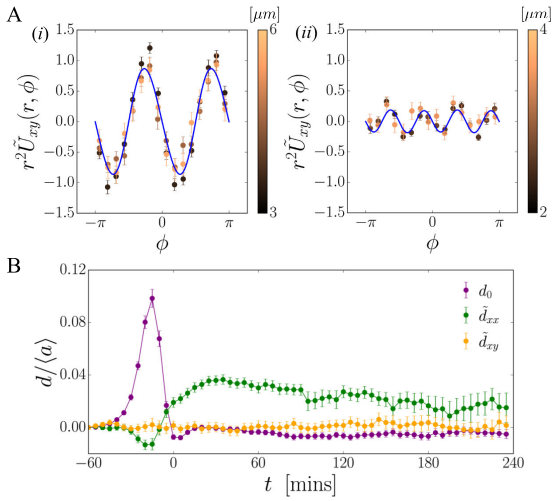

Figure 2: (A) The fit of linear elastic theory to the measured strain field around cell divisions at (A.*i*) the peak of inflation $t = -20$ [min] and (A.*ii*) after division $t = 30$ [min]. Each data point shows the average strain field in polar bins and the error bars are the standard deviation over these bins. (B) The normalised force dipole components generated by a cell division as a function of time d_{ij}, divided by the average cell area $\langle a \rangle$.

Here, r is the radial distance from the force dipole located at the origin, and φ is the polar angle. The constant $\mathcal{N}$ depends on boundary conditions, with $\mathcal{N} = 0$ in an infinite stress-free system.

Can we account for the observed strain field U_{ij} with the strain field u_{ij} predicted by the linear elastic theory strain field? We can immediately recognize that the observed angular Fourier modes (Fig. 1 D and Ref. [2]) indeed coincide with the dependence of propagator elements on the polar angle ϕ. We next fit u_{ij} to the experimental data using four fitting parameters: the three components of force dipole normalized by the shear elastic constant $d_{ij} = D_{ij}/2K$, and the elastic constants ratio μ. Note that d_{ij} has units of area. We find that two-dimensional linear elastic theory can indeed well account for the strain generated by cell divisions, and we show the fit of the theory and the corresponding experimental data for *xy* traceless-symmetric strain component in Fig. 2 A. The collapse of experimental data from different radial distances r in Fig. 2 demonstrates that the radial decay of the strain field is consistent with the theoretically predicted $1/r^2$.

Finally, we measure the strain field at a time resolution of 5 min and perform the fit of the theory to extract the dynamics of the force dipole generated by the dividing cell from the fit parameters, see Fig. 2 B. As expected, the inflation preceding the division is associated with a strong isotropic force dipole component d_0. Following the division, however, d_0 rapidly vanishes, and simultaneously the traceless-symmetric component $\tilde{d}_{xx}$ becomes imprinted in the tissue. Following the strain field over several hours after the division we can estimate the relaxation time-scale over which the imprinted strain is dissipated to be $\tau_\alpha = 3.5 \pm 0.7$ hr, which can be understood as the fluidization timescale of the fruit fly wing epithelium.

An important implication of our work is that the *Drosophila* wing epithelium is a solid whose fluidization time τ_α is not negligible on the developmental timescales. For example, large-scale shape changes that the wing undergoes during eversion occur on a similar timescale of several hours. Therefore, a relevant physical picture of the *Drosophila* wing epithelium on these intermediate timescales is that of a glassy material, or as is sometimes put forward in glass literature, a solid that flows.

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2.23 Mechanochemical feedback underlying Hydra regeneration

SUGANTHAN S. AND MARKO POPOVIĆ

Hydra regeneration Hydra is a freshwater organism that has a simple body plan. It consists of two layers of epithelia, which enclose a fluid filled lumen. The epithelia contain actin muscle fibers, which span the entire tissue and undergo contraction upon activation through calcium signaling. The actin fibers have a nematic symmetry and are well aligned throughout the animal, with perpendicular orientation of the fibers in the two epithelial layers. The fiber pattern contains several topological defects of total charge $+2$: one at the head, one at the foot, one at the tip and two at the base of each tentacle, see Fig. 1.

Hydra exhibits remarkable regeneration properties. A tissue fragment excised from the body of an adult animal can fully regenerate in about two days. During the regeneration process, the tissue fragment initially folds into a spheroid, undergoes repeated contractions due to muscle activation and finally forms the head on one side and foot on the opposite side, breaking the symmetry. The formation of the head is marked by the appearance of a +1 defect of the actin fiber pattern. This raises a question: how does the regenerating Hydra organise and stabilise the +1 defect? Namely, in a passive nematic liquid crystal on a spherical shell, the equilibrium state consists of four defects with topological charge +1/2.

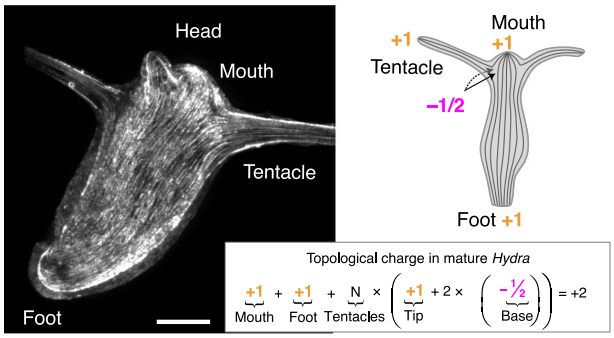

Figure 1: Pattern of actin fibers in Hydra observed in experiment (left) and summarised in a cartoon (right). Adopted from Ref. [1].

Experiments show that the future head of the Hydra, and the corresponding +1 defect in the pattern of actin fibers, is formed in the region of the tissue that exhibits repeated large stretching, observed very early in the regeneration. This suggests that a coupling between the actin fibers, the tissue strain field comprised of the cells and the extra-cellular matrix. Moreover, it is known that a morphogen called *Wnt* plays an important role in the head formation. It has been observed that up-regulation of *Wnt* or grafting a tissue fragment treated with *Wnt* onto a host tissue triggers the formation of additional heads in the animal centered around a +1 defect in the actin fiber pattern. On the other hand, when tissue stretching is reduced by placing the animal in isotonic conditions, where osmolarity of the environment matches that of the lumen, literature reports that expression of *Wnt* is suppressed, and we found that under these conditions the +1 defect becomes unstable and resolves into a pair of separated +1/2 defects. This type of experiment has two implications: it suggests that expression of *Wnt* is mechanosensitive and that *Wnt* is required to maintain a stable +1 defect. All these observations form a mechano-chemical feedback loop outlined in Fig. 2. Although some components of this loop have not yet been directly tested in experiments, here we consider them as a hypothesis to be explored, and for this we build a mechano-chemical model Hydra regeneration.

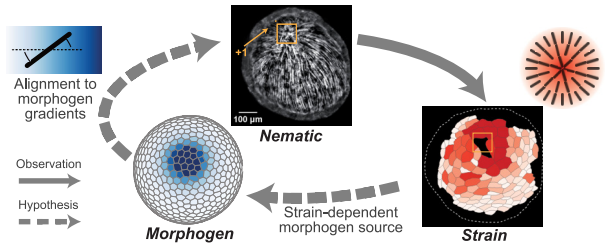

Figure 2: Mechano-chemical feedback loop we propose to explain the robust and flexible regeneration of Hydra.

Mechano-chemical model We first had to develop a mechano-chemical model of the regenerating Hydra epithelia that accounts for all components of the proposed feedback loop. For this, we designed a new type of vertex model of a deformable epithelial tissue, which encloses an incompressible lumen, but is otherwise allowed to deform. Cells are described as polygons, and internal mechanical forces on individual vertices are derived from the energy function

$$E = \sum_{c\in\text{cells}} \frac{K}{2}(A_c - A_c^0)^2 + \sum_{b\in\text{bonds}} \Lambda_b l_b + \sum_{c\in\text{cells}} \frac{\Gamma_c}{2} P_c^2 + \sum_{b\in\text{bonds}} \beta l_b (1 - \hat{n}_1.\hat{n}_2) + \mu V_{\text{lumen}} \qquad (1)$$

where the first three terms describe cell area elasticity, bond tension and cell perimeter elasticity, respectively. The fourth term penalises bending between two neighbouring cells with $\hat{n}_1$ and $\hat{n}_2$ denoting the normal vectors of cells c_1 and c_2 respectively, which share the bond

b. The last term imposes the constant lumen volume constraint where the lagrange multiplier μ is obtained by demanding $dV_{\text{lumen}}/dt = 0$.

Stresses due to activation of the actin fibers are oriented in each cell c along the a nematic unit tensor $\boldsymbol{q}_c$ that represents local fiber orientation. Generated active stress $\boldsymbol{\sigma}_c = -\zeta(t)\boldsymbol{q}_c$ in each cell is implemented by a set of active forces $\vec{\boldsymbol{f}}_{c,v}$ acting on each of the cell vertices v [2]. Here, $\zeta(t)$ is the activation function effectively representing calcium signalling, which we do not explicitly model here.

Finally, dynamics of each of the vertices is set by the total force acting on the vertex $\gamma d\vec{\boldsymbol{r}}_v/dt = -\partial E/\partial \boldsymbol{r}_v + \sum_c \vec{\boldsymbol{f}}_{c,v}$ where the sum is taken over all cells containing the vertex v.

We next introduce a morphogen number field N_c in each cell c that follows the dynamics according to

$$\frac{dN_c}{dt} = D \sum_{c,c' \in b} l_b(\phi_{c'} - \phi_c) - r_- N_c + f(\epsilon_c) \qquad (2)$$

where the first term corresponds to diffusion between two neighbouring cells c and c' that have morphogen concentrations ϕ_c and $\phi_{c'}$, respectively, with concentration defined by $\phi_c = N_c/A_c$. r_- is the morphogen degradation rate, and morphogen production depends on cell area strain through a response function $f(\epsilon_c)$ that is activated by cell area strain ϵ_c.

We close the feedback loop by coupling the cell nematic with the morphogen field as follows,

$$\frac{d\boldsymbol{q}_c}{dt} = \frac{1}{\tau_q}\langle \boldsymbol{q} \rangle_c + \alpha(\boldsymbol{\nabla}\phi_c \otimes \boldsymbol{\nabla}\phi_c)^{ST} + \lambda(\boldsymbol{q}_c)\boldsymbol{q}_c \qquad (3)$$

where the first term denotes the nearest neighbour alignment interaction at rate $1/\tau_q$ and the second term corresponds to alignment along the direction of morphogen gradient where α determines strength of the alignment and the superscript ST refers to the symmetric traceless component.

Simulations of Hydra regeneration We simulate the early regeneration of a Hydra tissue fragment, starting as a spheroid with a large region of disordered nematics that originates from the tissue excision and folding. We simulate the large-scale muscle contractions, characteristic for the Hydra tissues, by modulating the active stress magnitude $\zeta(t)$ over time. These stretching events occur on average about once per hour and last for about five minutes. We estimated most of the model parameters from either direct experimental observations or literature, and we explored the phase space of the two remaining parameters: morphogen alignment strength α and strain threshold ϵ_{th} that specifies the cell area strain required to initiate morphogen production. We find that our model can indeed robustly reproduce the formation of stable $+1$ nematic defect co-localized with the morphogen production region, see Fig. 3 and Ref. [2], and we can reproduce this behavior across a broad range of model parameters.

To further test the relevance of the mechano-chemical feedback loop in Hydra regeneration our collaborators constrained the regenerating Hydra in a narrow channel. Strikingly, when the initial fiber orientation was perpendicular to the axis of the channel the regeneration was frustrated, multiple $+1$ defects in the fiber pattern formed, and eventually multi-headed animals would emerge from the channel. We simulated the geometrically frustrated Hydra tissues by a narrow channel in our model and we found that such constraint is indeed sufficient to enable stabilization of multiple $+1$ defects, if the tissue aspect ratio imposed by the channel exceeds a critical value that we obtain in simulations. The results of this study are presented in Ref. [3].

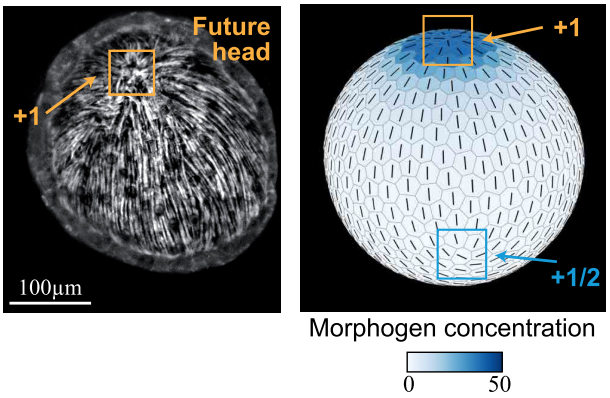

Figure 3: Actin fibers organise into a stable $+1$ nematic defect during the regeneration. Experimentally observed pattern of actin fibers is show on the left and an example of our model simulation rerpoducing the pattern is show on the right. Blue color indicates simulated concentration of morphogen, which co-localizes with the $+1$ nematic defect.

Besides accounting for our direct experimental observations, the mechano-chemical feedback loop proposed in our work is an appealing explanation as a mechanism for Hydra head regeneration due to its robustness in generating a stable $+1$ nematic topological defect, as well as its flexibility that stems from the fact that the feedback is entirely self-organized and does not require external driving or input. All reported results are the outcome of a close collaboration with the group of Kinneret Keren, which we now are continuing both to experimentally test specific interactions in the proposed feedback loop, and to theoretically examine corresponding emergent phenomena.

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2.24 Flocking by turning away

SUCHISMITA DAS, MATTEO CIARCHI, AND RICARD ALERT

Flocking — the self-organized collective motion of active agents — is ubiquitous in nature [1]. It takes place in many systems across scales, from bird flocks to bacterial colonies and to cytoskeletal filaments driven by molecular motors. Flocking is a landmark phenomenon that launched the field of active matter [2, 3]. As originally conceived in the Vicsek model, flocking arises through alignment interactions among the active agents, which align similarly to spins in the XY model. Alignment-based flocking was experimentally realized using synthetic active colloids, where the alignment interactions have either hydrodynamic, electric, or magnetic origin [4–6].

However, multiple recent works showed that flocking can also emerge without explicit alignment interactions — a situation that might be more common in nature than standard alignment interactions. For example, robots in a swarm benefit from collision-avoidance interactions. Similarly, several types of motile cells undergo contact inhibition of locomotion — a behavior whereby they repolarize away from collisions. Yet, cell layers have been observed to flock. How do cells flock despite interacting via contact inhibition of locomotion? What types of orientational interactions lead to flocking?

Here, we discovered a mechanism whereby self-propelled particles flock despite turning away from one another [7]. This finding is surprising because turn-away interactions are intuitively expected to prevent and destroy orientational order. We showed that this mechanism of flocking requires repulsion between the particles, which is also surprising given that the foundational Vicsek model has no repulsion at all.

We discovered this mechanism of flocking when analyzing experiments by our collaborators Jie Zhang and Ziqi Zhou at the University of Science and Technology China and Jing Yan at Yale. The experiments consist of self-propelled Janus colloids, which are silica spheres with a metal-coated hemisphere [8]. These particles are suspended in water and placed between two electrodes (Fig. 1(a)). They sediment into a two-dimensional layer and are driven by an electric field, which induces electric dipoles in each hemisphere (orange in Fig. 1(b)). These dipoles causes the particles to self-propel (black in Fig. 1(b)) and to interact via electrostatic repulsive forces (purple in Fig. 1(b)). Moreover, because the dipoles on the front repel more strongly than those on the rear, the particles interact via torques that reorient one particle away from another (green in Fig. 1(b)). Strikingly, as either the particle density (area fraction) or the self-propulsion speed increase, the system transitions from an isotropic to a polar flocking state (Figs. 1(c) and (d)).

To understand the origin of flocking in this system, we developed a microscopic model for the electrostatic interactions between the particles, which give rise to the following forces and torques:

$$\boldsymbol{F}_{ij} = \frac{3}{4\pi\epsilon}\frac{(d_\mathrm{h}+d_\mathrm{t})^2}{r_{ij}^4}e^{-r_{ij}/\lambda}\,\hat{\boldsymbol{r}}_{ij}, \tag{1}$$

$$\boldsymbol{\Gamma}_{ij} = \frac{3\ell}{4\pi\epsilon}\frac{d_\mathrm{h}^2-d_\mathrm{t}^2}{r_{ij}^4}e^{-r_{ij}/\lambda}\,\hat{\boldsymbol{n}}_j\times\hat{\boldsymbol{r}}_{ij}, \tag{2}$$

where ϵ is the dielectric permittivity of the solvent, $\boldsymbol{r}_{ij}=\boldsymbol{r}_j-\boldsymbol{r}_i$ is the distance vector, $d_\mathrm{h}>0$ and $d_\mathrm{t}<0$ indicate the effective dipole strengths of the head and tail hemispheres, respectively, and $\ell=3R/8$ is the dipole off-center distance, with $R=1.5$ μm being the particle radius. The exponential factor reflects the screening effect from the electrodes separated by $\lambda=120$ μm. The torque in Eq. 2 turns a particle with orientation $\hat{\boldsymbol{n}}_j$ away from the interparticle distance vector $\hat{\boldsymbol{r}}_{ij}$.

We write Langevin equations for the translational and rotational motion of particle i as

$$\frac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t} = v_0\hat{\boldsymbol{n}}_i(\theta_i)+\frac{\boldsymbol{F}_i}{\xi_\mathrm{t}}+\sqrt{2D_\mathrm{t}}\,\boldsymbol{\eta}_i^\mathrm{t}(t);\quad \boldsymbol{F}_i=\sum_{j\neq i}\boldsymbol{F}_{ji}, \tag{3a}$$

$$\frac{\mathrm{d}\theta_i}{\mathrm{d}t} = \frac{\Gamma_i}{\xi_\mathrm{r}}+\sqrt{2D_\mathrm{r}}\,\eta_i^\mathrm{r}(t);\quad \Gamma_i=\sum_{j\neq i}\boldsymbol{\Gamma}_{ji}\cdot\hat{\boldsymbol{z}}, \tag{3b}$$

where v_0 is the self-propulsion speed, $\hat{\boldsymbol{n}}_i=(\cos\theta_i,\sin\theta_i)$ is the orientation of particle i, ξ_t and ξ_r are the translational and rotational friction coefficients, respectively, and $\boldsymbol{\eta}_i^\mathrm{t}(t)$ and $\eta_i^\mathrm{r}(t)$ are Gaussian white noises with strengths given by the translational and rotational diffusivities D_t and D_r, respectively.

We performed Brownian dynamics simulations of this model, which reproduced the flocking transition. Because we knew the values of all microscopic parameters from our previous work [9], we were able to build a phase diagram that can be quantitatively compared to experiments. The phase boundary obtained from simulations (blue line in Fig. 1(e)) was quantitatively close to the experimental results (points in Fig. 1(e)). By running simulations at area fractions higher than in the experiments, we found that the flocks crystallized. These flocking crystals are formed due to particle repulsion, and hence they are active counterparts of Wigner crystals formed through electrostatic repulsion in electron gases.

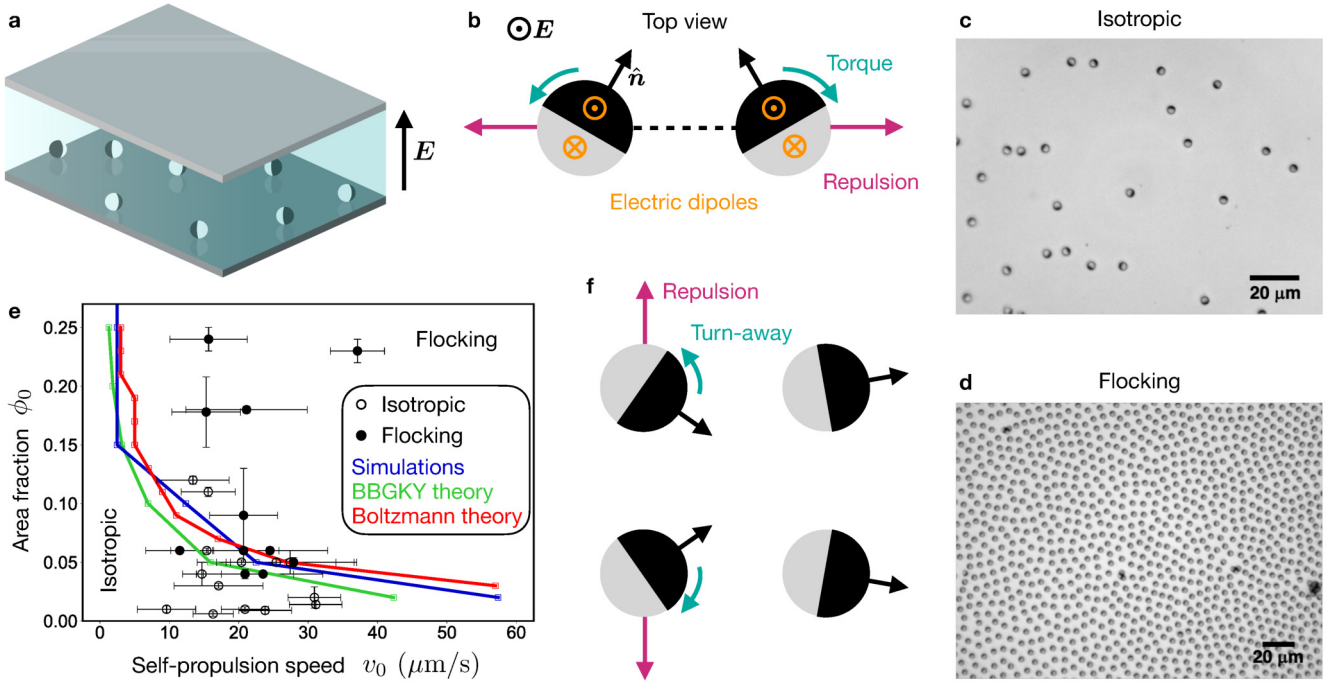

Figure 1: **Flocking of metal-dielectric Janus colloids. (a)** Schematic of the experimental setup. **(b)** Top view of two Janus particles in an electric field $\boldsymbol{E}$ that induces dipoles of opposite orientation and different magnitude (orange) on the head and tail hemispheres. This leads to particle self-propulsion along the direction $\hat{\boldsymbol{n}}$ (black), and to interparticle forces (purple) and torques (green). Torques rotate particles away from the direction of the interparticle distance (dashed line). **(c,d)** The system forms an isotropic gas at low area fraction and self-propulsion speed (c), and it flocks at high area fraction and speed (d). **(e)** Phase diagram of the flocking transition. Points show the experimental data. The lines indicate the phase boundaries that we predict via our simulations and two theory approaches. Error bars are s.d. **(f)** Schematic representation of how the combined effects of turn-away interactions (green) and repulsion (purple) produce effective alignment.

To understand the emergence of flocking, we coarse-grained the microscopic model using two types of kinetic theory: one based on the Smoluchowski equation and the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy known from the theory of liquids, and another one based on the Boltzmann equation for dilute gases. These two approaches allowed us to quantitatively predict the macroscopic collective behavior of the system based on its microscopic description. Strikingly, the flocking transition predicted by both approaches (green and red lines in Fig. 1(e)) are quantitatively consistent with our simulation and experimental results.

Moreover, these derivations revealed the mechanism of flocking. Our results showed that repulsion between the particles is essential: It prevents particles from turning away too much by pushing them apart during scattering events, thus creating an effective alignment (Fig. 1(f)).

In conclusion, our work identified a new mechanism of flocking, which might provide insights into how cells move collectively despite turning away from one another. Moreover, our work motivates further research into flocking crystals, which feature both positional and orientational order.

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2.25 Frictiotaxis

PETER HAMPSHIRE AND RICARD ALERT

In development, homeostasis and disease, cells migrate following environmental gradients. In particular, cells can follow gradients in substrate stiffness— a process called durotaxis [1,2]. So far, durotaxis has been mostly studied in cells that adhere to the substrate. To migrate, adherent cells use their actomyosin cytoskeleton to generate forces, which are then transmitted to the underlying substrate through molecular anchor points known as focal adhesions. Focal adhesions are supposed to be crucial for durotaxis as they enable cells not only to transmit traction forces but also to sense substrate stiffness. However, several cell types like various cancer and immune cells exhibit a mode of migration, often known as amoeboid migration, which does not involve focal adhesions [3]. In fact, most cell types switch to this migration mode under confinement [4]. However, whether cells lacking focal adhesions can respond to mechanical gradients is largely unknown [5].

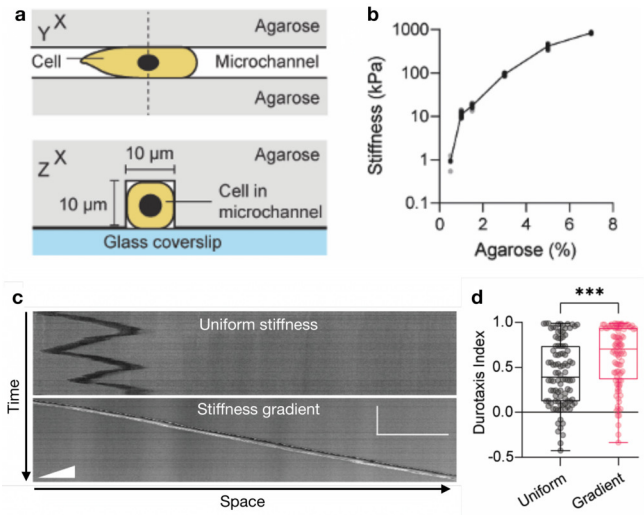

Figure 1: **Adhesion-independent durotaxis.** **a**, Cross-sectional schematics of the microchannel assays. **b**, Agarose gel stiffness increases with agarose concentration. **c**, Kymographs (space-time diagrams) of representative cells migrating in channels of uniform or graded stiffness. Cells reverse their direction often in uniform channels, but they migrate more persistently in a stiffness gradient, thus exhibiting durotaxis. Scale bar, 50 µm (horizontal), 50 min (vertical). **d**, Quantification of durotaxis. The durotaxis index is defined as $(d_{\text{up}} - d_{\text{down}})/(d_{\text{up}} + d_{\text{down}})$, where d_{up} and d_{down} are the distances travelled by the cell up and down the channel, respectively. $n = 100$ cells; two-tailed Mann-Whitney test; $^{***}P \leq 0.001$ (exact: $P = 0.0003$).

Here, we discovered that cells migrating without focal adhesions can perform durotaxis by following gradients in substrate friction— a process that we called frictiotaxis [6]. First, to answer whether amoeboid cells can perform durotaxis, our experimental collaborators A. Shellard and K. Weißenbruch in the lab of R. Mayor at UCL developed non-adhesive microchannels with tunable stiffness. The channels have one side made of glass coated with polyethylene glycol (PEG), and 3 sides made of agarose gel (Fig. 1a), whose stiffness is controlled by the agarose concentration (Fig. 1b). In these channels, Walker 256 carcinosarcoma cells did not form focal adhesions and performed amoeboid migration. Yet, these cells exhibited biased migration up the stiffness gradient, which shows that amoeboid cells can perform durotaxis (Figs. 1c and 1d).

To explain how these cells were able to durotax, we hypothesised that stiffer regions offer higher friction. Cell-wall friction can have multiple origins, including fluid lubrication forces and non-specific molecular interactions between transmembrane proteins and the channel walls.

To investigate this hypothesis, we considered a physical model for amoeboid migration which treats the actomyosin cortex as an active gel. The model imposes force balance:

$$\xi v = \partial_x \sigma. \tag{1}$$

The left-hand side represents cortex-substrate friction proportional to the cortex velocity $v(x)$ and the coefficient ξ. The right-hand side represents the forces arising from cortical tension $\sigma = \eta \partial_x v + \zeta c$, which has two contributions: viscous stresses with viscosity η, and myosin-generated contractility proportional to the myosin concentration c and the coefficient $\zeta > 0$. In turn, myosin is advected by cortical flows and diffuses with diffusivity D, thus satisfying:

$$\partial_t c + \partial_x (cv) = D \partial_x^2 c, \tag{2}$$

with no-flux boundary conditions $\partial_x c(\ell_\pm) = 0$ at the cell ends located at $x = \ell_\pm$. The cells ends move according to the cortical flow: $\mathrm{d}\ell_\pm/\mathrm{d}t = v(\ell_\pm)$. In addition, changing the cell length $L(t) = \ell_+(t) - \ell_-(t)$ around a reference L_r is opposed by an elastic force with stiffness k: $\sigma(\ell_\pm) = -k(L - L_\mathrm{r})/L_\mathrm{r}$.

This model captures amoeboid migration in the following way. An unpolarised cell, which has a uniform myosin concentration in the cortex, increases cortical contractility upon confinement [4]. Thus, when placed in a channel, the cell contracts (Fig. 2a, left). Contractility also triggers an instability whereby myosin accumulates on one side, which becomes the cell rear (Fig. 2a, right, Figs. 2c and 2d). Depending on how it breaks symmetry spontaneously, this concentration profile drives cell migration either left or right (Fig. 2a).

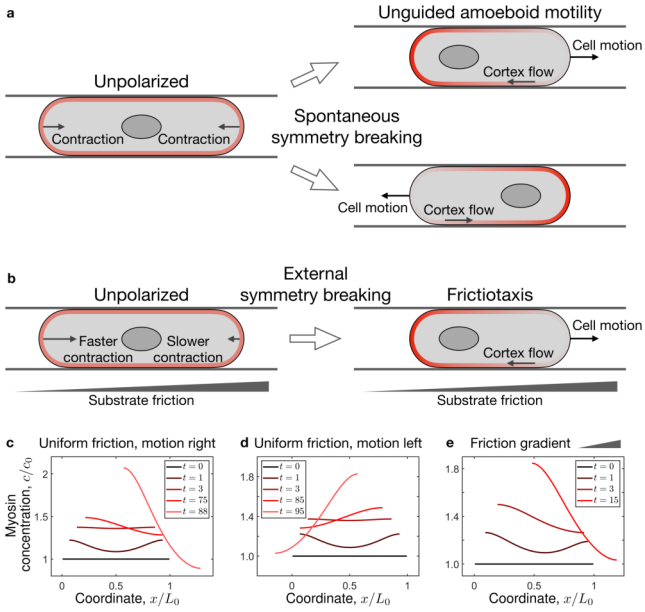

Figure 2: **Proposed mechanism for frictiotaxis. a**, In uniform channels, cell contraction is symmetric. Therefore, unpolarised cells break symmetry spontaneously, and hence they move either left or right. Red coloring represents myosin concentration. **b**, On a friction gradient, cell contraction is asymmetric, which leads to cell migration towards higher friction. **c-e**, Numerical solutions of the model showing these mechanisms of symmetry breaking. The time unit is $10^{-4}L_0^2/D$, where L_0 is the initial cell length.

What happens if there is a friction gradient? We consider again an unpolarised cell (Fig. 2b, left), which contracts upon being confined. In this case, the cell end at lower friction contracts faster than the end at higher friction. Hence, myosin accumulates faster at the low-friction side, which thus becomes the cell rear. The cell therefore moves up the friction gradient— a behavior that we call frictiotaxis. We demonstrated this mechanism of symmetry breaking in numerical solutions of the model with a linear friction profile $\xi(x)$ (Fig. 2e).

To test the idea that friction underlies adhesion-independent durotaxis, our collaborators performed two additional experiments. First, they used lateral force microscopy (LFM) to measure the friction on the agarose gel. Indeed, they found that the friction coefficient increased with substrate stiffness (Fig. 3a), as also predicted by theoretical models [7]. Therefore, a gradient in stiffness produces a gradient in friction, which can affect cell migration even in the absence of focal adhesions. Second, to disentangle the effects of stiffness and friction, our collaborators created channels with uniform stiffness but a friction gradient. This was done by coating the glass with a gradient of PEG and bovine serum albumin (BSA). Both substances are non-adhesive and provide different friction (Fig. 3b). In these channels, cells exhibited biased migration up the friction gradient, which directly confirmed frictiotaxis in experiments (Figs. 3c and 3d).

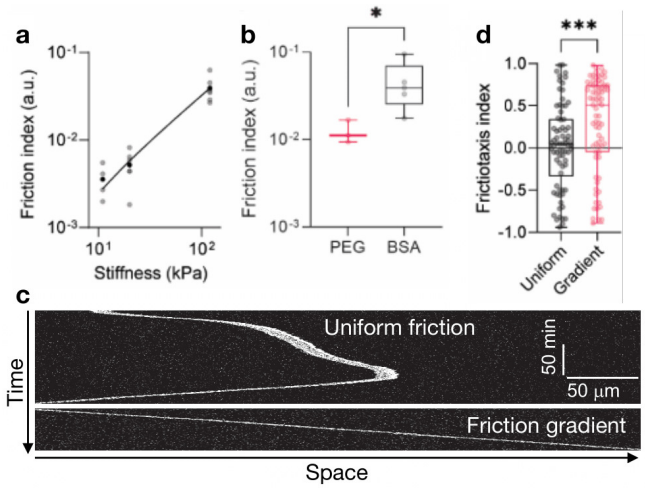

Figure 3: **Frictiotaxis. a**, The friction index of agarose gels measured by LFM increases with stiffness. **b**, Friction index of PEG- or BSA-coated glass; $n = 3$ (PEG); $n = 5$ (BSA); two-tailed Mann-Whitney test; $^*P \leq 0.05$ (exact: $P = 0.0357$). **c**, Kymographs (space-time diagrams) of representative cells migrating in channels of uniform or graded friction. Migration is more persistent up friction gradients. **d**, Quantification of frictiotaxis. The frictiotaxis index is defined equivalently to the durotaxis index in Fig. 1. $n = 74$ cells; two-tailed Mann-Whitney test; $^{***}P \leq 0.001$ (exact: $P = 0.0010$).

Altogether, our results reveal that amoeboid cells can perform durotaxis thanks to friction forces, because friction is correlated with substrate stiffness. Our findings also reveal frictiotaxis as a new mode of guided cell migration. These results imply that, in addition to the well-known chemical guidance (chemotaxis), amoeboid migration can also be guided by mechanical cues. Our findings have implications for cell migration during development, immune response and cancer progression, which usually takes place in confined environments that favour amoeboid migration. Investigating how adhesion-independent durotaxis and frictiotaxis manifest in such *in vivo* settings poses an interesting challenge for future work.

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2.26 Spatiotemporal Characterization of Active Transport Processes

YANIS BAOUCHE, AND CHRISTINA KURZTHALER

Introduction Microorganisms utilize various swimming strategies to optimize their survival and efficiently explore their environment. Through adaptation to their surroundings, bacteria, algae and other animalcules have developed elaborate self-propulsion mechanisms that allow achieving diverse biological functions. Mimicking these navigation techniques, progress has recently been achieved in the domain of nano-technology through the design and fabrication of robots, finding numerous applications in bioremediation and medicine [1].

A widely-studied biological exemplar is the bacterium *Escherichia Coli*. Its biochemistry and genetics have been extensively studied, but predicting its dynamics has remained a challenge. The gait of *E. Coli* is dictated by the persistent motion due to the synchronized movement of several flagella and sudden changes of its swimming direction induced by flagella unbundling; this locomotion pattern is typically referred to as "run-and-tumble" (RT) motion [Fig. 1**A**] [3, 3]. On the synthetic side, the paradigmatic example represents the phoretic *Janus* colloid. Its dynamics can be quantitatively described by the "active Brownian particle" (ABP), whose orientation performs rotational diffusion [4]. These systems display intriguing out-of-equilibrium dynamics, where the translational-rotational coupling introduces nonlinear features. These both render the theoretical description of the spatiotemporal dynamics challenging and reveal a plethora of new interesting physical phenomena. Here, we will focus on the description of the RT dynamics of *E. coli* [3,3] and discuss the dynamics of ABPs under stochastic orientational resetting, as a tool to guide ABPs towards a specific target [5].

Theoretical framework To describe the inherently stochastic nature of tumbling and orientational resetting (referred to as renewal events), we use a renewal theory. It consists of two equations coupling the probability $P(\boldsymbol{r},t)$ of the active agent to have displaced a distance $\boldsymbol{r}$ during lag time t and the probability density per unit time $Q(\boldsymbol{r},t)$ for a renewal event:

$$Q = Q_1 + \int_{\mathbb{R}^2} \mathrm{d}\boldsymbol{l} \int_0^t \mathrm{d}t' Q(\boldsymbol{r}-\boldsymbol{l}, t-t') T(t') \mathbb{P}(\boldsymbol{l}, t'),$$
$$P = P_0 + \int_{\mathbb{R}^2} \mathrm{d}\boldsymbol{l} \int_0^t \mathrm{d}t' Q(\boldsymbol{r}-\boldsymbol{l}, t-t') S(t') \mathbb{P}(\boldsymbol{l}, t'),$$

where $Q_1(\boldsymbol{r},t)$ and $P_0(\boldsymbol{r},t)$ represent the probability for the first renewal event per time and the probability that no renewal event has happened until t, respectively, accounting for the non-equilibrium steady state. Further, $T(t')$ is the probability density that the renewal event happens at t' and $S(t') = \int_0^{t'} \mathrm{d}s T(s)$ is the probability that the time to the next renewal event exceeds time t'. Further, $\mathbb{P}(\boldsymbol{l},t')$ denotes the propagator for the dynamics between two renewal events. The motion of a RT particle or an ABP under orientational resetting can then be described by appropriately choosing $T(t')$ and $\mathbb{P}(\boldsymbol{l},t')$.

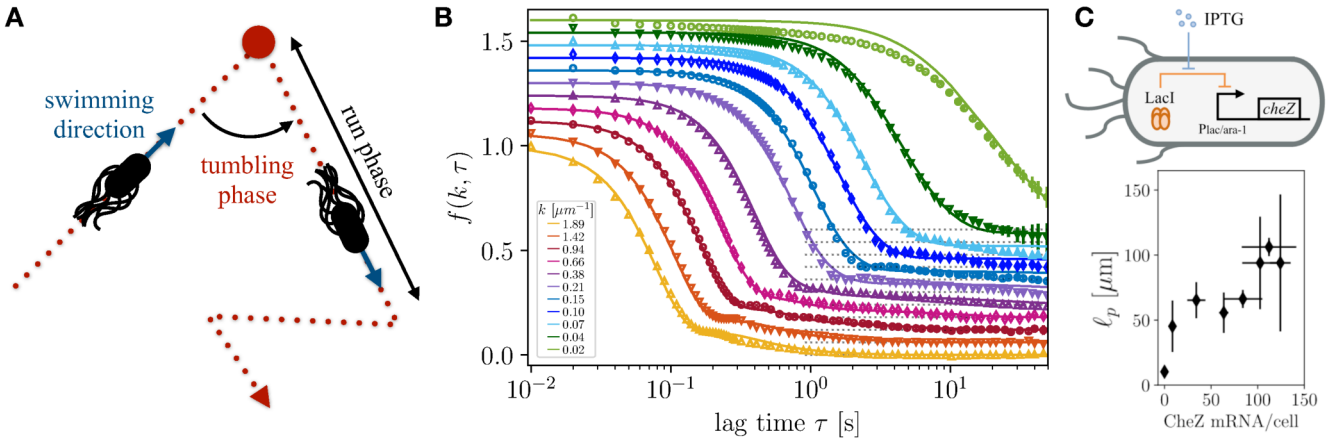

Figure 1: **Characterization of the run-and-tumble dynamics of** *E. Coli* **bacteria. A** Sketch of the run-and-tumble mechanism. **B** Intermediate scattering functions $f(k,\tau)$ as a function of lag time τ for several wavenumbers k. Symbols and lines represent experimental measurements and our theoretical predictions, respectively. **C** Sketch of the engineered cell and measurement of its persistence length ℓ_p as a function of CheZ mRNA per cell.

Run-and-tumble dynamics of *E. Coli* To study the bacterium's dynamics, we compute the intermediate scattering function (ISF) via a Fourier transform of the probability density $P(\boldsymbol{r},t)$: $f(\boldsymbol{k},t) = \int \mathrm{d}\boldsymbol{r} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} P(\boldsymbol{r},t)$, where $\boldsymbol{k}$ denotes the wave vector. This quantity allows characterizing the bacterium's dynamics at lag time t and length scales $2\pi/|\boldsymbol{k}|$. It represents the fundamental ingredient for analyzing experimental measurements of *E. Coli* obtained via the high-throughput method differential dynamics microscopy (DDM). It circumvents the need of single-particle tracking in three dimensions, limited by statistical accuracy and typically short trajectories, and provids access to data over long time and large length scales required to quantify the cell's swim gait. In Fig. 1 **B**, we compare theoretical ISFs with experimental measurements and observe excellent agreement over several orders in length and time scales, thus quantitatively bridging for the first time small-scale directed swimming and macroscopic diffusion. Fitting the experiments to our renewal theory, we were able to extract the kinetic parameters, such as the tumbling rate, the average speed, and the translational diffusivity.

We further employed our framework to study the relation between molecular mechanisms of the flagella motor and the swimming gait. Therefore, we use an engineered strain, whose *cheZ* gene has been deleted. By tuning the concentration of Isopropyl β-d-1-thiogalactopyranoside (IPTG) during cell growth, the expression of *cheZ* can be restored. Our results show that the persistence length ℓ_p, i.e., the length the bacteria travels through persistent swimming before tumbling, one can see in increases with the concentration of *cheZ* mRNA inside the cell [Fig. 1 **C**]. This demonstrates the role of *cheZ* in tuning the tumbling rate of *E. coli* (as the swim speed remains unaffected) and reveals, for the first time, a controlled transition from a perpetual tumbling to a smooth swimming behavior.

Stochastic orientational resetting While bacteria have evolved chemotactic strategies by, for example, exploiting the molecular machinery discussed above, it is an important task to develop methods that can guide their synthetic counterparts towards a specific target. As a first step towards quantifying such dynamics, we consider an ABP that randomly resets its orientation along a predetermined direction. Assuming that the run times are exponentially distributed with mean $1/\lambda$, allows us to define the reduced rate $\Lambda = \lambda/D_{\mathrm{rot}}$, characterizing the relative importance of the resetting mechanism with respect to rotational diffusion. The interplay of these two mechanisms can be quantified in terms of the propagator $P(\boldsymbol{r},t)$, which we compute semi-analytically using our renewal approach [Fig. 2]. We find that for agents resetting along the $x-$direction it becomes most prominent at $\Lambda = 0.5$, where the distribution at short times has a tail to the left, accounting for agents reorienting due to rotational diffusion. As the agent resets more often, its position distribution becomes increasingly skewed towards the $x-$ direction. Our analytical results show that at long times the distributions approach Gaussians with a finite drift velocity.

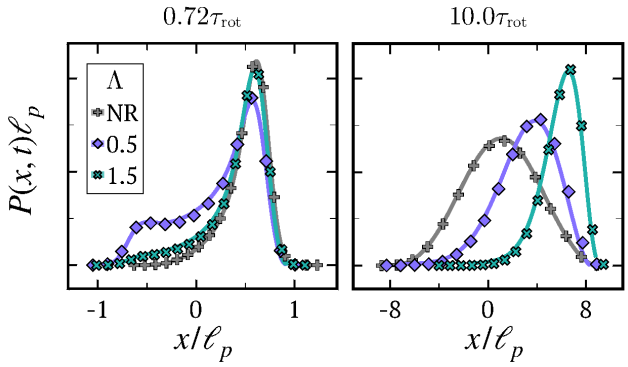

Figure 2: **Stochastic orientational resetting.** Marginal of the probability distribution, $P(x,t)$. The Péclet number is $\mathrm{Pe} = 10$, τ_{rot} denotes the rotational relaxation time, and l_p is the persistence length. NR corresponds to the non-resetting case. Theory and simulation are shown with lines and symbols, respectively.

Conclusion Our work lays the foundation for studying the swimming gait of various microorganisms, beyond the RT behavior. We further note that the ability of microorganisms to respond to chemical fields or gradients, through quorum sensing or chemotaxis, is a vital part of their foraging and survival strategy. Extensions of our theory on orientational stochastic resetting, together with spatiotemporally resolved DDM, opens a new way for quantifying such response at the population level. Future work will leverage this framework towards unraveling first-passage-time properties of active agents.

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2.27 Flow Through Porous Media at the Percolation Transition

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Introduction Transport processes through complex media play fundamental roles in diverse areas, ranging from ancient irrigation systems to modern technological applications, such as oil recovery from tight reservoirs, water filtration, and processing of polymeric materials, to geophysics, where pollutants contaminate rocky materials, to biology. The latter involves the circulation of blood through microvascular networks, microbial motion through wet soil and dense tissues [1], and molecular transport in the interior of crowded cells, to name a few. In these heterogeneous environments, fluid flow encounters intricate surface topographies [2,3] as well as highly disordered porous structures with many dead-end pockets and corners, yielding numerous regions of stagnant flow alongside a few pores of rapid fluid streams [4]. These intricate flow fields can generate hydrodynamic dispersion of individual consitutents [5] and are strongly affected by complex fluid properties. Thus, the interplay of hydrodynamic flows and complex geometries represents an exciting topic at the interface of fluid mechanics and statistical physics with several fundamental questions for various fields remaining still open.

One important aspect, that has remained a puzzle to date, concerns the behavior of Stokes flow through dense porous media, where phenomenological laws, such as Darcy's law, break down. Important contributions to understanding fluid flow through dense environments come from percolation theory, which analyzes system properties that emerge when the density of obstacles, called packing fraction ϕ, reaches a critical point ϕ_c, i.e. when the obstacles form a cluster that spans the entire porous media, preventing the fluid flow through it. In the proximity of such a density, called percolation threshold, geometrical properties and transport properties become universal. In the context of fluid flow, Ref. [6] predicted that the flow rate Q through a porous media obeys $(\phi_c - \phi)^\alpha$ with $\alpha \approx 5/2$ by mapping the fluid flow through the porous media onto a discrete random flow network. This prediction could provide fundamental physical insights from first principles, yet to date a numerical or experimental verification of this scaling prediction has remained out of reach.

Power-law behavior of flow through porous media at the percolation transition In this work, we model the porous medium as a two-dimensional rectangle of width H in which obstacles are represented by disks of the same radius a that are randomly distributed and may overlap. The spatially-varying fluid velocity and pressure fields, $\mathbf{u}$ and p, obey the Stokes equations: $\mu\nabla^2\mathbf{u} - \nabla p = \mathbf{f}$ and $\nabla\cdot\mathbf{u} = 0$, where μ denotes the fluid viscosity and $\mathbf{f}$ is an external force applied to mimic pressure-driven flow. No-slip boundary conditions are imposed at the surface of the discs. The equations are solved numerically using a finite-element scheme and to assure statistical accuracy we generate at least 30 independent samples for every ϕ.

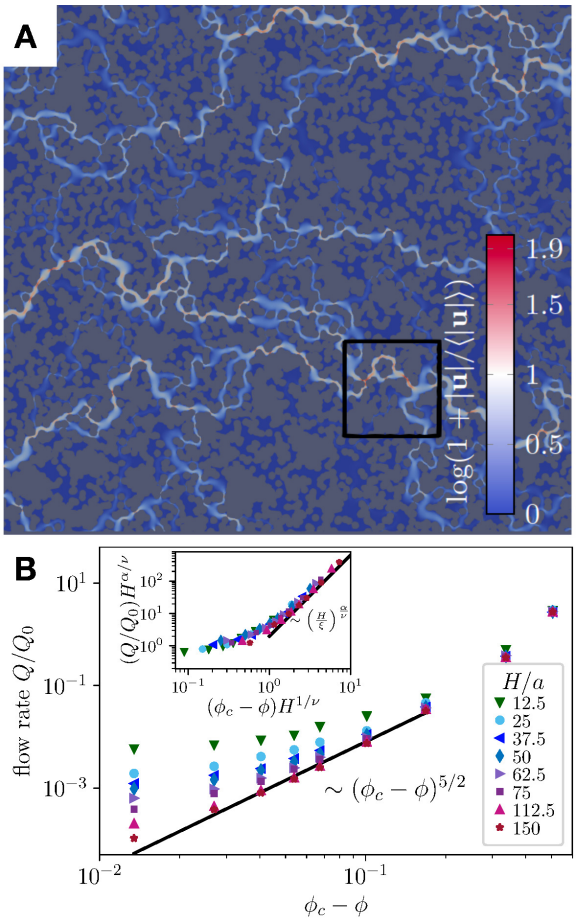

Figure 1: **Flow through a porous medium. A** Velocity field of a low-Reynolds-number flow through a two-dimensional Lorentz gas composed of overlapping discs with radius a. **B** Flow rate Q as a function of packing fraction ϕ for different system sizes of height H. (*Inset*) Finite-size scaling of the flow rate. Here, ϕ_c denotes the critical packing fraction, ξ is the correlation length, and the critical exponents are $\alpha = 5/2$ and $\nu = 4/3$.

Most importantly, our results demonstrate a power-law scaling of the flow rate as the percolation threshold ϕ_c is approached, $Q \sim (\phi_c - \phi)^\alpha$. Fitting the data for a porous channel of width $H/a = 150$ and $\phi_c - \phi \lesssim 0.02$, yields an exponent of $\alpha \simeq 2.44 \approx 5/2$ [4][Fig. 1], which agrees with the prediction of Halperin et al. [6]. Our results for very dense environments show that the underlying flow field becomes highly heterogeneous, characterized by a few fast streams transporting fluid across

the porous medium, which allows mapping the behavior of the macroscopic flow to a discrete flow network as done in [6]. We further stress that this critical behavior in principle holds for infinitely large systems ($H \to \infty$) and is expected to be recovered for finite system sizes that are larger than the correlation length ξ of the void space, $H \gtrsim \xi$. Our results show that deviations appear for smaller system sizes, $H/a \lesssim 100$, where the curves of the flow rate bend and the power-law behavior becomes rounded. To interpret these results we perform a finite-size scaling ansatz. In particular, we note that the scaling prediction for the flow rate can be expressed by $Q \sim \xi^{-\alpha/\nu}$ with $\nu = 4/3$ [6]. For small systems, $H \ll \xi$, H assumes the role of ξ, modifying the prediction to $Q \sim H^{-\alpha/\nu}$ for $\phi \to \phi_c$. Using the ansatz

$$Q/Q_0 = H^{-\alpha/\nu} f(H^{1/\nu}(\phi_c - \phi)),$$

with scaling function $f(x) = \text{cte.}$ for $H \ll \xi$ and $f(x) \sim x^{\alpha}$ for $H \gg \xi$, nicely collapses our data covering sizes of $12.5 \leq H/a \leq 150$ at high packing fractions [Fig. 1**B**(inset)]. Our results thus suggest that ξ is the relevant length scale of our system, and the expected scaling with exponent $\approx 5/2$ is only smeared out by finite-size effects.

Kinetic energy of the velocity field Analyzing the distribution of the kinetic energy of the fluid, denoted as $E = |\mathbf{u}|^2/|\mathbf{u}|^2_{\max}$, in the porous media, we find a power-law scaling $\text{PDF}(E) \sim E^{-\beta}$ with $\beta \approx 0.9$ as the percolation threshold is approached. The latter remains persistent over several decades in the range of $\sim 10^{-9}E - 10^{-1}E$ [Fig. 2], i.e. for small kinetic energies. These energies are mostly found in the dead-end-pores of the medium, where the flow consists of a cascade of viscous eddies with a rapidly decreasing intensity and consequently energy [inset of Fig. 2]. This is consistent with predictions for viscous corner flows in terms of asymptotic, self-similar solutions [7], implying that the $\text{PDF}(E)$ at low E is predominantly influenced by a collection of viscous eddies within dead-end channels. Therefore, we anticipate that the power-law behavior emerges due to the self-similar nature of the individual viscous eddies and the extended power-law represents a collection of these.

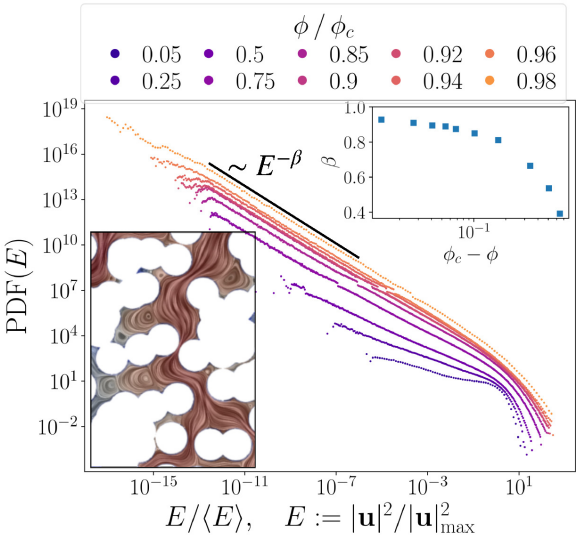

Figure 2: **Probability density function of the kinetic energy E.** Different colors correspond to different packing fractions ϕ and ϕ_c denotes the critical packing fraction. (*Lower inset*) Eddies in dead-end-pores. (*Upper inset*) Fitted exponent of the PDF vs. ϕ.

Conclusions and outlook Our findings on Stokes flow through porous media demonstrate a power-law scaling of the macroscopic flow rate with an exponent $\approx 5/2$ at the percolation threshold, thus confirming analytical predictions by Halperin et al. [6]. Moreover, our study has provided a firm foundation for understanding Stokes flow through dense porous media via a finite-size scaling analysis. Looking ahead, our findings lay the foundation to study the physics of complex fluids in disordered media and unraveling power-law behaviors for e.g., non-Newtonian or active fluids. Importantly, our theoretical framework enables the study of the interplay of fluid shear, features of active transport, and the density of the porous media, which are expected to lead to rich physics that could be paramount for the survival strategies of microorganisms.

Acknowledgements The authors gratefully acknowledge computing time granted by the Center for Information Services and High-Performance Computing at the TU Dresden. P. Das acknowledges funding via the Alexander von Humboldt foundation.

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2.28 Robust cytoplasmic partitioning by solving an intrinsic cytoskeletal instability

MELISSA RINALDIN, ALISON KICKUTH, ADAM LAMSON, BENJAMIN DALTON, AND JAN BRUGUÉS

In early embryos, cell boundaries are established by rapid cleavage divisions that robustly organize the cytoplasm into progressively smaller cellular compartments. Strikingly, the compartmentalization of the cytoplasm can occur before [1] or without [2] the formation of a new plasma membrane, raising the question of how boundaries between cytoplasmic compartments can be robustly maintained in the absence of physical barriers. The formation and division of these compartments rely on microtubule asters that define their boundaries [3] and dynein activity that transports organelles towards the compartment center [4]. Microtubule asters grow via self-amplifying microtubule growth or autocatalytic nucleation, the nucleation and branching of microtubules from existing ones [5]. When asters enter in contact, the aster-aster interface is thought to be stabilized by components that provide local inhibition to microtubule nucleation and growth, creating robust boundaries that guide cytokinesis [6]. However, it is unclear how local inhibition in combination with autocatalytic growth can lead to stable and robust boundaries [7].

We investigated cytoplasmic partitioning in X. laevis frog egg extracts. Undiluted cytoplasm obtained by crushing frog eggs at high speed self-organizes into distinct compartments that are not separated by cell membranes, similarly to syncytial systems (Fig. 1A). To quantify the formation of compartment boundaries we measured the microtubule density profile using EB1-mApple (Fig. 1B). Near the interface of the compartments, the microtubule profiles decay consistent with local inhibition at the antiparallel microtubule overlap. These profiles suggest that the interaction between the two asters can be minimally described by a network of two autocatalytic, or self-amplifying, loops interacting via local inhibition, resulting in the following equation:

$$\frac{d}{dt}\rho_i = \mp v_p \partial_x \rho_i + \alpha \frac{\rho_i}{1+(\rho_1+\rho_2)/\rho_s} - \theta\rho_i - \lambda \frac{\rho_1\rho_2}{\rho_1+\rho_2}, \quad (1)$$

In this equation, $i = 1, 2$ and refers to the two asters, v_p is the polymerization velocity, θ the microtubule turnover, α is a parameter related to the autocatalytic growth, λ modulates the inhibition between asters, and ρ_s is a density of microtubules that indicates the saturation of microtubule nucleation due to depletion of nucleators as they bind to microtubules. We measured v_p by tracking the plus ends of the microtubules and θ using single molecule microscopy of sparsely labelled tubulin dimers. To estimate α, we used the initial explosive growth of microtubules close to the center of the compartments, far from the interaction zone between asters. Finally, we estimated the local inhibition λ by measuring the slopes of the density of microtubules at the interaction zone. With all parameters fixed, we plotted the theoretical aster density profiles and observed that they quantitatively agree with the experiments (Fig. 1B). Surprisingly, we found that both theory and agent based simulations predict that the temporal evolution of these boundaries is unstable. This instability is generally expected from local inhibition and self-amplification alone; however, it disagrees with the robustness of cytoplasmic organization observed in embryos and cycling extracts. One possible explanation for this apparent inconsistency between theory and experiments is that the time needed to develop such instability may be larger than the cell cycle time, which drives the disassembly of the microtubule asters prior to the assembly of mitotic spindles. To test whether the cell cycle prevents the development of the instability, we arrested cytoplasmic extracts in interphase. We observed that compartments that initially formed with a well-defined boundary as in the control condition, started coarsening by means of the microtubule asters invading each other and fusing, consistent with the aster invasion predicted by our theory (Fig. 1C).

Our results suggest that the cell cycle duration can determine whether invasion events occur and thus regulate the patterns of cytoplasmic partitioning. To further investigate this dependence, we experimentally quantified the invasion time as a function of the aster mass difference. The invasion time decays as the mass difference between the asters increases. This trend is also perfectly captured by a parameter-free prediction of the theory (Fig. 1D black line). Asters with large mass differences invade in a few minutes. Interestingly, asters with small mass differences—that represent the situation in living embryos where compartments are highly uniform—have an invasion time comparable to the cell cycle time. We wondered if there were regimes in the parameter space that could prevent this instability, independently of the cell cycle timing. To this end, we performed a linear stability analysis of Eq. 1, leading to the stability criterion:

$$\theta > \alpha/(1+2\rho_{int}/\rho_s), \quad (2)$$

where ρ_{int} is the density of microtubules where the two asters intersect. Surprisingly, the stability of the compartment boundaries critically depends on a competition between the autocatalytic rate and microtubule turnover, and not on the strength or the shape of the lo-

cal inhibition term. When the autocatalytic term dominates over turnover, the boundary they form will always be unstable. Conversely, if turnover dominates over autocatalytic growth, the density of microtubules decreases from the center of the compartment. In this regime, the boundary created as the two asters interact will be stable, but the compartments will be generally smaller with a size defined by the decay length scale of the microtubule density. Consistent with the instability we measured, extracts fall in the unstable regime of the stability criterium. These results show that the stability of compartments can be achieved by modulating microtubule nucleation and dynamics, independently of cell cycle timing.

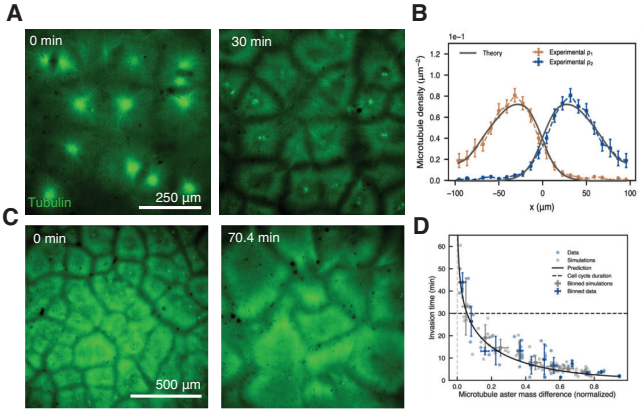

Figure 1: (A) Live imaging of cycling extract showing cytoplasmic partitioning by microtubule asters over multiple cell cycles. Microtubules are labeled by Alexa640-tubulin and shown in green. (B) Microtubule density profile of two asters as they start interacting, obtained by measuring the density of growing plus ends in the growth direction in the region where the asters interact. (C) Live imaging of interphase-arrested cytoplasmic extract showing microtubule aster invasion. Aster invasion results in the fusion of cytoplasmic compartments. (D) Invasion time plotted against initial mass difference between the asters, showing that asters with small mass differences take longer to invade than asters with large mass differences. Cell cycle time of the frog embryo is plotted for comparison.

Using a theory for aster-aster interactions, and experiments in extracts , we revealed that cytoplasmic partitioning prior to cytokinesis is an intrinsically unstable mechanism. This instability originates from a competition between microtubule autocatalytic growth and turnover. Despite this inherent instability, we demonstrate that precise cell cycle timing renders this compartmentalization dynamically stable, resulting in remarkably robust partitioning of the cytoplasm. To find the proper geometric center, cells read the geometrical boundaries of the embryo using unstable microtubule waves that reach the cortex [3]. This instability imposes a delicate balance between the waves of autocatalytic growth and the cell cycle timing. The cell cycle duration needs to be slow enough for waves to read the geometry of the cell but fast enough that compartments do not fuse. The cell cycle also needs to be synchronous across compartments to avoid invasion events, as seen in Xenopus egg extracts. This synchronization is fundamental at the beginning of development when the timescale of completing membrane ingression is longer than a single cell cycle duration. As development progresses and ingression of the cell membrane is completed, the cell membrane can block invasion events and ensure correct multicellularity. In organisms that do not require early cellularization, it is not necessary to immediately read the cell geometry. Instead, smaller and stable asters that compartmentalize a shared cytoplasm can slowly divide and fill up the embryo space prior to cellularization. In this situation, there is no need to rely on unstable autocatalytic processes or to have a perfectly synchronized cell cycle as the compartments remain stable.

This work presents a novel integration of Turing-like mechanisms with biological oscillators, contributing to the understanding of pattern formation dynamics. We explore a network characterized by local self-amplification (autocatalytic growth of the asters) and local inhibition. This network is unstable, however, when properly modulated with the cell cycle oscillator, it gives rise to dynamically stable and robust states. This combination of unstable networks with oscillators unlocks a realm of previously unexplored unstable regimes, yielding dynamically stable patterns endowed with remarkable traits such as rapid spatial coverage and flexibility. Departing from the traditional characterization of robust Turing networks as stable [7], our study illuminates the potential of coupling unstable mechanisms with oscillators. Overall, our research exemplifies how precise temporal tuning of biological oscillators can govern spatial patterning and cellular organization, highlighting how physical and geometrical constraints influence the evolution of self-organization mechanisms.

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2.29 Impossible Ecologies

YU MENG, SZABOLCS HORVÁT, CARL D. MODES, AND PIERRE A. HAAS

Introduction. Half a century ago, May [1] introduced ideas from random matrix theory into theoretical ecology to show that, perhaps contrary to expectations, coexistence in large ecological communities is overwhelmingly likely to be unstable. Ever since, theoretical ecologists have striven to identify those ecological structures that stabilise actual ecological communities. In this context, the role of the detailed network structure of competitive, mutualistic, and predator-prey interactions between species remains largely unknown, perhaps because it does not allow the direct statistical description that would make it amenable to random-matrix-theory approaches.

Here [2], we study this detailed network structure by exhaustive analysis of the stability and feasibility of steady-state coexistence in all ecological networks of $N \leqslant 5$ species [Fig. 1(a)]. We consider the simplest, Lotka–Volterra dynamics of these N species [Figs. 1(b),(c)], to which any ecological dynamics reduce in the vicinity of an equilibrium. Each network topology is thus determined by a vector $\boldsymbol{A}$ and a matrix $\boldsymbol{B}$, for which the Lotka–Volterra dynamics [Fig. 1(b)] have a single equilibrium of coexistence of all species, $\boldsymbol{x}_* = \boldsymbol{B}^{-1} \cdot \boldsymbol{A}$. This equilibrium is *feasible* if $\boldsymbol{x}_* \geqslant \boldsymbol{0}$ elementwise, and is *stable* if the dynamics return to this equilibrium under small perturbations, which is if and only if the eigenvalues of the Jacobian $-\boldsymbol{x}_*\boldsymbol{B}$ have negative real parts.

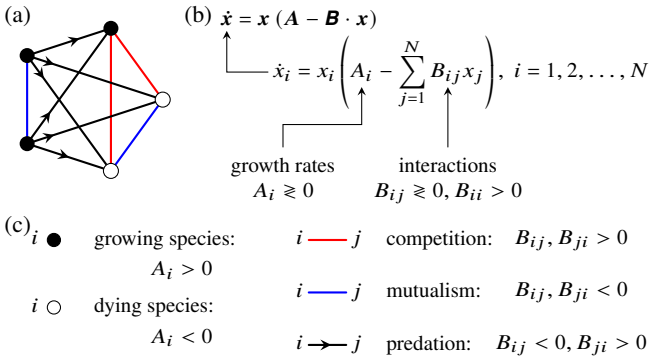

Figure 1: Lotka–Volterra ecological dynamics. (a) Example of a network topology on $N = 5$ species, defined below. (b) Mathematical definition of the Lotka–Volterra model on N species: The dynamics of the vector $\boldsymbol{x}$ of the population abundances of the N species are determined by the vector $\boldsymbol{A}$ of growth rates and the matrix $\boldsymbol{B}$ of interaction strengths. (c) The network topology or *ecology* is defined by the signs of $A_i \gtrless 0$ and $B_{ij} \gtrless 0$ for $i \neq j$, which define competitive, mutualistic, and (directed) predator-prey interactions between species.

To address the effect of network topology on coexistence, we computed probabilities $\mathbb{P}$ of stable and feasible coexistence by fixing a network topology and by sampling its parameters, i.e., the absolute values of the elements of $\boldsymbol{A}$ and $\boldsymbol{B}$, independently and uniformly from the uniform $\mathcal{U}[0, 1]$ distribution.

Impossible ecologies. There are 10 network topologies on $N = 2$ species (Fig. 2). Of these, 4 are trivial [Fig. 2(b)] because (at least) one species dies on its own and has only deleterious interactions with other species. The abundance of this species must decrease, so there cannot be stable and feasible coexistence of all species. The remaining 6 ecologies [Fig. 2(a)] are non-trivial, but, interestingly, one ecology ["obligate mutualism", highlighted in Fig. 2(a)] is an *impossible ecology*: The conditions for stable and feasible coexistence for this network topology lead to a non-trivial contradiction [2].

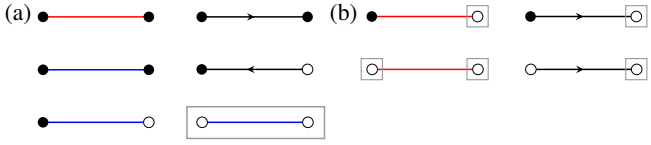

Figure 2: Two-species ecologies. (a) List of the six non-trivial network topologies on $N = 2$ species: One topology ("obligate mutualism", highlighted) is an *impossible ecology* in which stable and feasible coexistence is non-trivially impossible. (b) List of the four trivial ecologies on $N = 2$ species: Some species (highlighted) are dying on their own and have only deleterious interactions, precluding stable and feasible coexistence of all species.

Irreducible ecologies. There are 70 non-trivial network topologies on $N = 3$ species. The corresponding probabilities of stable and feasible coexistence [Fig. 3(a)] vary over orders of magnitude. In particular, this probability is much lower for one particular ecology [highlighted in Fig. 3(a)]. This is an instance of another interesting type of ecology: *Irreducible* ecologies are those non-trivial ecologies that are possible, but all subecologies of which are trivial or impossible. There are 6 such ecologies for $N = 3$, shown in Fig. 3(b). The decomposition into trivial and impossible subecologies is illustrated there for one irreducible ecology. There are also 4 impossible ecologies for $N = 3$, shown in Fig. 3(c); again, the conditions for stable and feasible coexistence lead to a non-trivial contradiction for these topologies [2].

Extensions of ecologies. A topology is *possible* if it allows stable and feasible coexistence for some parameter values. A topology is an *extension* of another topology if the second can be obtained from the first by removing one species and its interactions with the remaining species. With these definitions, the importance of impossible and irreducible ecologies is highlighted by the following theorem:

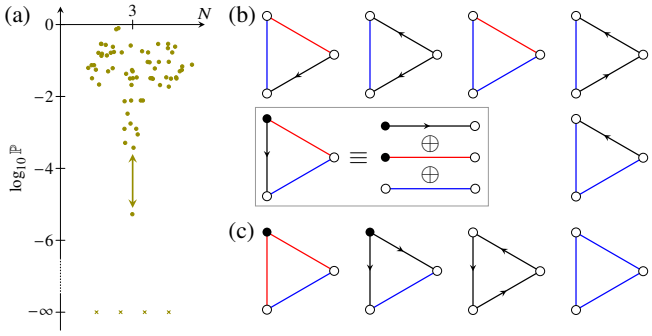

Figure 3: Three-species ecologies. (a) Swarm plot of the probability $\mathbb{P}$ of stable and feasible coexistence for all 70 non-trivial ecologies of $N = 3$ species. For impossible ecologies, $\log_{10} \mathbb{P} = -\infty$. (b) *Irreducible* ecologies of $N = 3$ species; the decomposition into impossible or trivial two-species subecologies is given for one. (c) Impossible ecologies of $N = 3$ species.

Theorem [2]. Any non-trivial extension of a possible ecology is itself possible.

Indeed, an immediate corollary of this theorem is that the possibility of stable and feasible coexistence is determined completely by the classification of irreducible and impossible ecologies.

The first step towards this classification is enumeration of non-trivial ecologies. There is a bijection between our network topologies and directed graphs with self-loops [2]. This allows computationally efficient enumeration of these ecologies using established tools from computational graph theory. As expected, the number of non-trivial ecologies undergoes a combinatorial explosion: For $N = 4, 5, 6$, there are 2340, 248 436, and 88 124 740 non-trivial network topologies, respectively.

Still, computational classification of irreducible and impossible ecologies was possible for $N = 4, 5$ by implementing the classification code in C++, using the `eigen` library for small matrix operations.

Already for $N = 4$, the probabilities of stable and feasible coexistence [Fig. 4(a)] vary over more than ten orders of magnitude. Remarkably however, there are at most 11 impossible ecologies [insets in Fig. 4(a)] among the 2340 non-trivial network topologies. There is only this upper bound on the number of impossible ecologies because the strategy [2] deployed to prove that certain ecologies with $N = 2$ or $N = 3$ are impossible does not suffice to show that these topologies, which our numerical sampling suggests to be impossible, are actually impossible.

Extending these computations, we obtain upper bounds on the fraction of impossible, irreducible, and non-trivial non-extension (i.e., impossible or irreducible) ecologies of $N \leqslant 6$ species [Fig. 4(b)]. Remarkably, our numerical results suggest that these ratios decrease at least exponentially as the number N of species increases. In other words, the possibility of stable and feasible coexistence in a general ecology is determined by a tiny subset of all network topologies! This is our main result and shows that the details of the network topology are hugely important for stability and feasibility of coexistence.

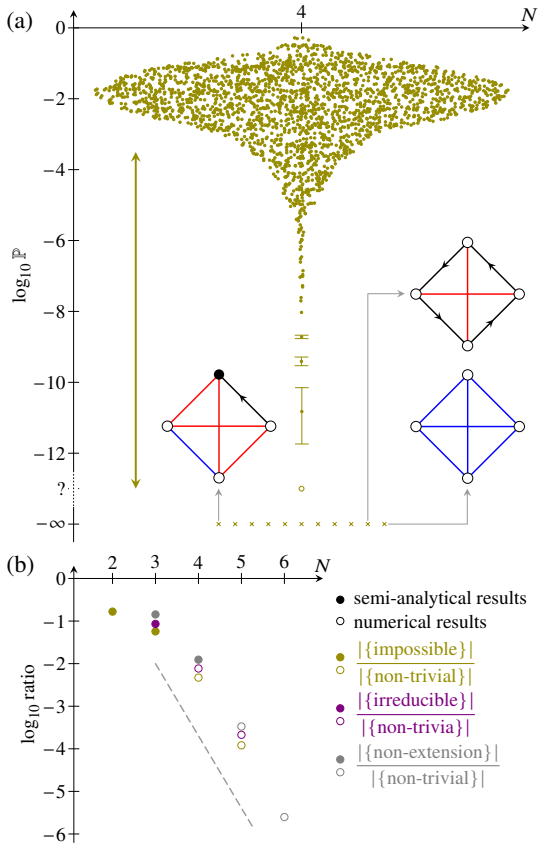

Figure 4: Larger ecologies: rareness of irreducible and impossible ecologies. (a) Swarm plot of the probability $\mathbb{P}$ of stable and feasible coexistence for all 2340 non-trivial ecologies of $N = 4$ species. Impossible ecologies ($\log_{10} \mathbb{P} = -\infty$) were identified based on numerical computations; there is no analytical proof of their impossibility at this stage. The question mark (?) indicates an ecology for which the probability $\mathbb{P}$ could not be computed, but which was shown to be impossible by finding parameter values allowing stable and feasible coexistence by non-uniform numerical sampling of feasible equilibria. Error bars are 95% confidence intervals larger than the plot markers. Insets: examples of four-species ecologies asserted to be impossible. (b) Plot of the fraction of impossible, irreducible, and non-extension ecologies against N, based on semi-analytical and numerical results, suggesting that these ratios decrease exponentially as N increases (dashed line).

Applications. The importance of these details is stressed further in applications of our exhaustive enumeration to classical questions of theoretical ecology, such as assembly of ecological communities or perturbations of ecological interactions [2].

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2.30 Mechanics of poking a cyst

SHIHENG ZHAO AND PIERRE A. HAAS

Introduction. Just as one pokes fruits to evaluate their ripeness and hence their comestibility, indentation of cysts (spherical monolayers of polarised cells surrounding a fluid-filled lumen) by microbeads attached to AFM cantilevers [1, Fig. 1(a)] quantifies their material properties. However, just as evaluation of the comestibility of the fruit of one's choosing relies on one's experience of the relation between poking force and indentation depth for a ripe fruit, quantification of these material properties relies on a physical model of the relation between the indentation force F and the indentation depth e.

The classical Pogorelov problem [Fig. 1(b)] of the indentation of an elastic shell of radius R and thickness $h \ll R$ by a point force provides such a mechanical model, predicting $F \sim e$ for $e \ll h$, and, for $e \gg h$, $F \sim e^{1/2}$ for an unpressurised shell ($p = 0$), but $F \sim e$ for a pressurised shell ($p \neq 0$) [2, Fig. 1(c)]. While the cells constituting a cyst are expected to respond elastically on the short timescales of indentation experiments, this model neglects physical effects such as nonlinear elastic contributions, the incompressibility of the lumen surrounded by the cells, or the pre-stress induced by cell contractility.

Here [3], we combine analytical calculations, scaling arguments, and finite-element simulations to show that these effects give rise to even new scaling exponents in the force-displacement relation of the Pogorelov problem. We conclude by finding signatures of these scaling exponents in cyst indentation data [1].

The purely nonlinear Pogorelov problem. We begin by solving the "purely nonlinear" Pogorelov problem. Our starting point is a general incompressible polynomial hyperelastic energy density,

$$W = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} C_{mn}(\mathcal{I}_1-3)^m(\mathcal{I}_2-3)^n, \tag{1}$$

where $\mathcal{I}_1, \mathcal{I}_2$ are the principal invariants of the right Cauchy–Green tensor of the deformation, and $C_{00} = 0, C_{10}, C_{01}, \ldots$ are material parameters. The leading terms in this expression constitute the Mooney–Rivlin density

$$W_1 = C_{10}(\mathcal{I}_1-3) + C_{01}(\mathcal{I}_2-3). \tag{2a}$$

For a thin elastic shell of thickness h, this reduces to the linear shell energy density

$$\hat{W}_1 = 4G_1 h\left(E^2 + \frac{h^2}{12}K^2\right), \tag{2b}$$

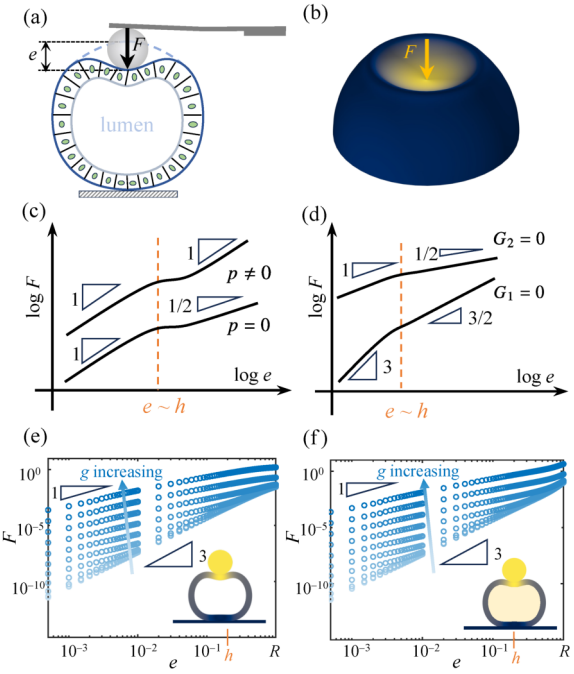

Figure 1: Mechanics of poking a cyst. (a) Indentation of a cyst consisting of a spherical monolayer of cells surrounding a fluid-filled lumen by a microbead attached to an AFM cantilever, yielding the relation between the poking force F and the indentation depth e. (b) Pogorelov problem: An elastic shell of radius R and thickness $h \ll R$ is indented by a point force F. (c) Scaling exponents in the force-displacement relation of the unpressurised ($p = 0$) and pressurised ($p \neq 0$) Pogorelov problems [2]. (d) New scaling exponents for the purely nonlinear unpressurised Pogorelov problem ($G_1 = 0$), different from the classical exponents ($G_2 = 0$). (e) Finite-element simulations for different values of $g \equiv G_1/G_2$ show that the scaling exponents for $e \lesssim h$ even persist for thick shells indented with a sphere (inset). (f) Further finite-element simulations show that these exponents persist for an incompressible lumen (shading in inset), too.

in which E and K are measures of the stretching and bending of the shell, respectively, and where $G_1 = C_{10} + C_{01}$ is the linear shear modulus. If $G_1 = 0$, the material is purely nonlinear, and Eq. (1) is led by

$$W_2 = C_{20}(\mathcal{I}_1-3)^2 + C_{11}(\mathcal{I}_1-3)(\mathcal{I}_2-3) + C_{02}(\mathcal{I}_2-3)^2. \tag{3a}$$

The corresponding shell theory is [3]

$$\hat{W}_2 = 16G_2 h\left(E^4 + \frac{h^2}{4}C^4 + \frac{h^4}{80}K^4\right), \tag{3b}$$

where $C \sim \sqrt{EK}$ couples stretching and bending. We call $G_2 = C_{20} + C_{11} + C_{02}$ the nonlinear shear modulus of the shell.

To solve the Pogorelov problem for this purely nonlinear shell theory, we use the geometric scalings from the classical Pogorelov problem to show that the energy of a purely nonlinear Pogorelov "dimple" is [3]

$$\mathcal{E}_2 \sim \begin{cases} G_2 e^4 h^2 R^{-3} & \text{for } e \ll h, \\ G_2 e^{5/2} h^{7/2} R^{-3} & \text{for } h \ll e\,(\ll R). \end{cases} \tag{4}$$

This is balanced by the work $\mathcal{W} \sim Fe$ done by the indenting force. It follows that $F \sim e^3$ for $e \ll h$ and $F \sim e^{3/2}$ for $e \gg h$. Importantly, these scaling exponents are different from those of the classical Pogorelov problem [Fig. 1(d)].

To verify these exponents, we performed finite-element simulations [3] within COMSOL MULTIPHYSICS for different values of $g \equiv G_1/G_2$. These results show how the scaling exponents transition from these new values to the classical ones as g increases. Remarkably, we do not only observe these exponents in the asymptotic limit $h \ll R$ of a thin shell indented by a point force assumed in our analytical calculations, but they also persist in the limit of a thick shell indented by a sphere [Fig. 1(e)] relevant for cyst indentation experiments. In fact, these exponents even persist, for experimentally relevant indentation depths comparable to the shell thickness, if a constraint imposing lumen incompressibility is added [Fig. 1(f)].

Pressure and pre-stress: Scaling arguments. This success of our scaling arguments suggests that we can extend them to pressurised and pre-stressed cysts. We focus on the scaling $e \ll h$ because we have observed those exponents in our finite-element simulations of thick cysts. The "dimple" formed by indentation has volume $V \sim e^2 R$, so the energy contribution from pressure is

$$\mathcal{E}_p \sim p e^2 R. \tag{5}$$

Pre-stress from cell contractility induces a pre-strain E_0 that replaces $E \to E + E_0$ in Eqs. (2b) and (3b). If $E_0 \ll E \sim e/R$, the previous scalings [Fig. 1(d)] continue to hold; if $e \ll E_0 R$ (and $e \ll h$), the energy of a linear or purely nonlinear Pogorelov dimple becomes [3]

$$\mathcal{E}_1 \sim \frac{G_1 h^2 E_0^{1/2} e^{3/2}}{R^{1/2}}, \qquad \mathcal{E}_2 \sim \frac{G_2 h^2 E_0^{5/2} e^{3/2}}{R^{1/2}}, \tag{6}$$

respectively. Hence there are three possible scalings for the force $F \sim \mathcal{E}/e$: $F \sim e^{1/2}$ (associated with pre-strain), $F \sim e$ (associated with pressure or linear elasticity), and $F \sim e^3$ (associated with nonlinear elasticity). Which exponent arises depends on which physical effect dominates the mechanics [Fig. 2(a)]. At small enough e, the first scaling must dominate, but other, larger exponents may take over as e increases and other physical effects begin to dominate [Fig. 2(a)]. In particular, transitions between scaling exponents correspond to changes of the dominant physical effect, and whether they do arise depends on the physical parameters $p, G_1, G_2, E_0, h/R$ of the problem [3].

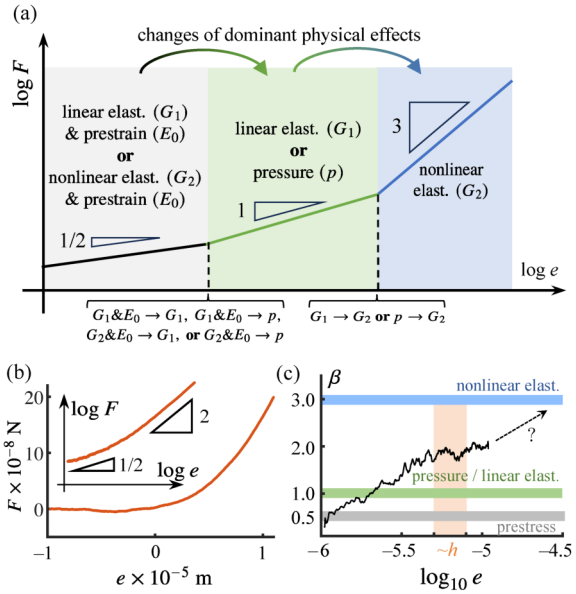

Figure 2: Scaling exponents for cyst indentation and experimental verification. (a) Force-displacement relation of a Pogorelov dimple with pressure p and pre-strain E_0. Depending on the physical parameters $p, G_1, G_2, E_0, h/R$, at different indentation depths, different physical effects dominate and different scaling exponents arise. (b) Example force-displacement relation from indentation of a cyst of MDCK cells [1]. Inset: same data on logarithmic axes, showing a scaling exponent increasing from $1/2$ to 2. (c) Plot of the local scaling exponent $\beta = \mathrm{d}(\log F)/\mathrm{d}(\log e)$, obtained by smoothing the raw data in panel (b). Horizontal lines emphasise the scaling exponents predicted for different dominant effects in panel (a).

Experimental verification. To verify these results, we reanalysed cyst indentation data from Ref. [1]. The force-displacement relation, plotted in Fig. 2(b), shows an exponent β increasing from $1/2$ to 2. The data thus feature the exponent $\beta = 1/2$ that we have predicted in the pre-strain dominated regime. Meanwhile, the local scaling exponent is still increasing at the end of the experimental curve [Fig. 2(c)]. Deeper indentations could confirm whether the scaling exponent would indeed increase from $\beta \approx 2$ to the predicted value $\beta = 3$, but are limited by the cantilever in the indentation setup [Fig. 1(a)]. Importantly however, observing $\beta > 1$ already signals a contribution of nonlinear elasticity, because our simulations of thick shells [Figs. 1(e),(f)] do not yield $\beta > 1$ at experimentally relevant indentation depths without nonlinear elastic contributions.

This confirms that cell contractility and nonlinear elasticity contribute to the mechanics of the cyst. Our results thus form the basis for inferring the mechanisms that set the mechanical properties of these cysts.

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2.31 Quasi-particle kinetics in compartmentalised systems

F. MEIGEL AND S. RULANDS

Understanding how fluctuations travel across different spatial scales is the fundament of theories of inanimate matter. For instance, in turbulent flows, velocity fluctuations generated at large scales travel down to the microscopic level where they eventually dissipate. Similarly, in systems near criticality, fluctuations self-similarly extend from the microscopic to the macroscopic scale, resulting in diverging thermodynamic response functions. These behaviors are elucidated by theoretical frameworks—such as renormalization group theory and coupled modes theory—that quantify the collective impact of all intermediate scales on the physical properties of interest.

In contrast, biological systems are structured as a distinct hierarchy of non-equilibrium processes that span vastly different spatial dimensions (Fig. 1(a)). At the molecular level, reactions occur within specialized subcellular structures called organelles, while cells organize into complex tissues and organs [1]. Unlike inanimate matter, biological systems have evolved explicit mechanisms to convey fluctuations and signals between these scales. For example, the decision of a cell to undergo apoptosis (programmed cell death) is orchestrated by complexes of apoptosis-regulating proteins, including Bax. Under stress conditions, Bax is recruited from the cytosol to the mitochondrial outer membrane (MOM) at a rate that reflects the cell's stress level. Once localized at the MOM, these proteins engage in stochastic dynamics that lead to the formation of pores. These pores then facilitate the release of cytochrome C from the mitochondria, irreversibly committing the cell to apoptosis. Furthermore, mitochondria are highly dynamic entities that continually undergo fusion and fission, causing fluctuations in the concentration of protein complexes on their membranes. This dynamic interplay enables a bidirectional propagation of fluctuations and signals between the molecular and organelle scales.

In this work, we demonstrated that compartmentalized systems possess an emergent degree of freedom whose kinetic characteristics are exploited by cells to make regulatory decisions [2]. We focussed on a representative class of compartmentalized stochastic systems in which stochastic processes are nested within interacting compartments. To this end, we integrated out probability fluxes between the microscopic and the compartment scale to derive an effective description of the time evolution of the probability that a randomly chosen compartment has a concentration c at a given time t,

$$\partial_t f(c,t) = \partial_c \left[F(c) + \partial_c \Phi(c)\right] f(c,t) + \partial_c^2 D(c) f(c,t) \quad (1)$$

Here, the first term on the right-hand side describes the deterministic drift of the probability density function. This drift happens with a velocity that is proportional to the deterministic force $F(c)$ and additional feedback from the compartment scales. This feedback is given by an additional effective interaction potential $\Phi = \Lambda \int \mathrm{d}c' f(c',t)(c'-\bar{c})^2$, which describes an attractive force to the mean in the concentration space. The second diffusive term on the right-hand side describes the dispersive spreading of f due to noise. In general, we showed that equations of the form of Eq. (1) exhibit a localization phase transition [3]. We showed that if interactions between compartments are long-range the probability density function localizes in concentration space. Analogous to localization phenomena observed in condensed matter physics, we refer to this localized mode as a quasi-particle.

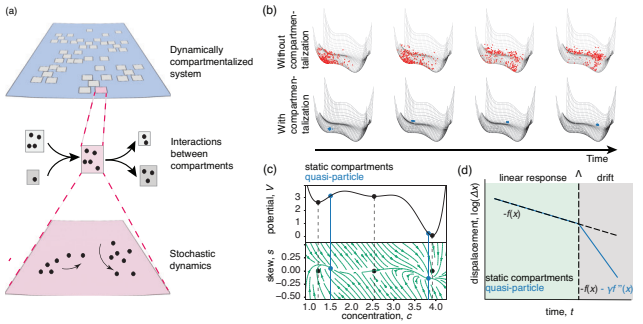

Figure 1: (a) Schematic illustrating the concept of a dynamically compartmentalized system. (b) Snapshots of a stochastic simulation illustrating the emergence of quasi-particle kinetics. (c) Exemplary fixed points and phase portrait of the quasi-particle kinetics for a tristable system. (d) Nonlinear response function of the quasi-particle.

Therefore, the time evolution of the stochastic multiscale system is effectively described by a single degree of freedom, which is the position of the quasi-particle in concentration space (Fig. 1(b)). The kinetics of the quasi-particle is effectively described in terms of its "position" x as the geometric median of the distribution of compartment concentrations, $f(c,t)$, and its "internal deformation" as the non-parametric skew, $s = \bar{c} - x$. In the limit of weak forces $F(c)/\Lambda \ll 1$ and weak noise $D(c) \to 0$ to the highest order in the derivatives of $f(c,t)$, the equations of motion for the quasi-particle read $\dot{x} = F(x) + \Lambda s$, and $\dot{s} = -\Lambda s - \gamma F''(x)$ (Supplemental Theory 2.6.). γ is a parameter that is proportional to $D(x)\Lambda^{-1}$, and for times much longer than the time scales much longer than Λ^{-1} it quantifies the width of the distribution $f(c,t)$. Therefore, the deterministic motion in concentration space is complemented by an effective drift proportional to the non-parametric skew s. This drift takes a value that expo-

nentially approaches a steady state given by the second derivative of the force $F(x)$. For time scales much longer than the time scale of the compartment dynamics, the equation of motion of the quasi-particle simplifies to

$$\dot{x} = F(x) - \gamma F''(x).. \quad (2)$$

With this equation of motion, we have reduced the dynamics of a high-dimensional multi-scale system to the time evolution of a single degree of freedom, x. The simplicity of the equation of motion allows graphical integration and thus offers an intuitive approach for predicting the emergent consequences of dynamic compartmentalization.

The dynamics of the quasi-particle defined by exhibit a qualitatively different behavior compared to non-compartmentalized systems. First, the stationary states of the quasi-particle position $\dot{x} = 0$ do not necessarily coincide with the fixed points of $F(x)$ (Fig. 1(c)). In general, since the quasi-particle distorts the force $F(x)$ on length scales smaller than its variance and deepens it on much longer length scales, the number of metastable states is reduced compared to the number of fixed points of $F(x)$. In equilibrium biochemical systems this implies that steady states do not coincide with the minima of the Gibbs free energy defined by the chemical reactions.

Dynamically compartmentalized systems exhibit distinct responses to perturbations. In particular, when examining the linearized response kinetics of the quasi-particle to perturbations in the force $F(x)$, two temporal regimes emerge. On short time scales, the response is dominated by a rapid relaxation of s to its steady state. In contrast, on time scales much longer than $1/\Lambda$, the dynamics become governed by the nonlinear characteristics of the force.

This behavior can be intuitively explained through a spring system analogy. When the position of the central mass is perturbed on time scales significantly shorter than the characteristic retardation time ($1/\Lambda$), the resulting deflection occurs independently of the positions of the other masses, similar to a point mass moving within a potential. Conversely, perturbations that occur on time scales much slower than the retardation time propagate between the masses, leading to a collective response that reflects the non-local properties of the potential.

We finally showed that cells make use of quasi-particle kinetics to decide their fate. To this end, our collaborators in the group of Philipp Mergenthaler at the Charité Berlin conducted experiments on the decision of cells to commit suicide (apoptosis). Apoptosis is of fundamental importance for cells to build complex tissues and to maintain their integrity. Based on the known biochemistry of the processes underlying apoptosis we predicted that in this case the quasi-particle kinetics would create a kinetic low-pass filter of fluctuations in cellular stress levels. To test this, we subjected cells to chemical stress signals over varying periods of time and measured the probability of cell death over time. As predicted by the kinetic low-pass filter property we found that indeed the cell-death decision was suppressed on short time scales and enhanced on long time scales.

Taken together, in this work we developed a general theory of multi-scale biological systems. These systems generically give rise to quasi-particles in concentration space with unique kinetic properties. We also showed experimentally that cells make use of these properties to control their fate. Our work sheds a new light on how cells process and interpret signals.

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2.32 Non-equilibrium quantum liquids of periodically driven fermions

LIKUN SHI, OLES MATSYSHYN, JUSTIN SONG, AND INTI SODEMANN

Abstract. This report summarizes results from Refs. [1–3], where we found that non-equilibrium driven quantum fluids of fermions can display additional emergent Fermi surfaces that are sharply different to those in equilibrium. Refs. [1, 2] showed that driven fermions in contact with a larger cold fermion system (i.e. a Fermion bath) reach a non-equilibrium state whose occupation of states is not the Fermi-Dirac distribution which has a single jump, but a new "stair-case" occupation function with multiple jumps (Fig. 1(a)). Each of these additional jumps leads to a new Fermi surface that would be absent in equilibrium (Fig. 1(a)). On the other hand, Ref. [3] found that driven fermions in contact with a larger bosonic system (i.e. a boson bath), reach a non-equilibrium state whose occupation is a non-analytic function of momentum with sharp "kinks" (Fig. 1(a)). These "kinks" define new non-equilibrium emergent Fermi surfaces with different universal properties compared to equilibrium ones. For example, the ripples induced by an impurity (Friedel oscillations) decay with a different power-law [3]. Remarkably, these new "kink" Fermi surfaces remain sharp even at finite temperature [3], a phenomenon with no analogue in equilibrium Fermi surfaces.

The problem of filling Floquet bands The Fermi surface is a central object in the understanding of quantum fluids of fermions in equilibrium. It plays a central role in a plethora of characteristic quantum behaviors of fluids of Fermions, ranging from the long-ranged ripples induced by an impurity (Friedel oscillations), to the oscillatory behavior of their physical quantities under magnetic fields (i.e. Shubnikov de-Haas effect), to their tendency to Cooper-pair superconductivity at low temperatures. Our studies are motivated by the following question: What is the fate of the Fermi surface in fermionic quantum fluids driven far from equilibrium by periodic driving?

An advantage of considering periodically driven Hamiltonians is that they retain a stroboscopic notion of energy (a.k.a. Floquet energy) and energy eigenstates (a.k.a. Floquet eigenstates). Therefore, just like we have a band-structure for electrons in crystals in equilibrium, there is a Floquet band-structure when their Hamiltonian is periodic in time (obtained, e.g., by simply shining coherent mono-chromatic light on them). However, a key challenge is that these bands should not be filled by the Fermi-Dirac distribution because the system is away from equilibrium. In Refs. [1–3] we have found remarkable answers for how to fill these Floquet bands in the case of fermionic systems coupled to either fermionic or bosonic baths.

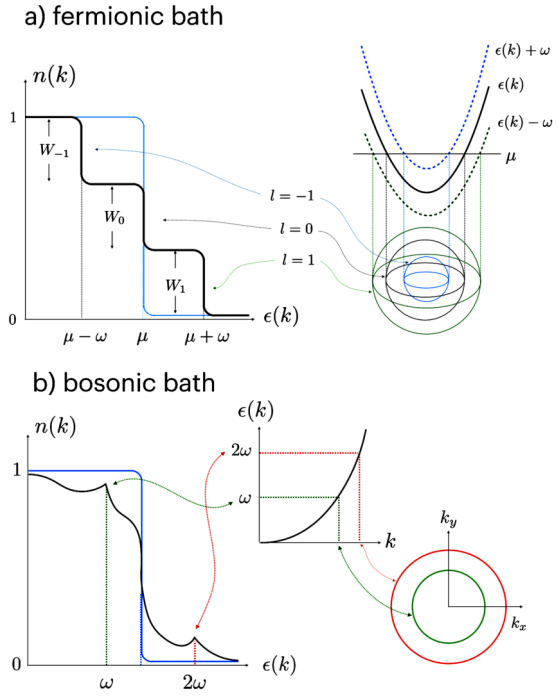

Figure 1:
a) Staircase occupation (black line) of fermions of a Floquet band coupled to a fermion bath at driving frequency ω, showing the principal step and the first two non-trivial steps, that lead to appearance of multiple Floquet Fermi surfaces enclosed inside each other (top right).
b) Non-equilibrium occupation (black line) of fermions of same Floquet band but coupled to a boson bath, which is a non-analytic function displaying cusps (bottom left), leading to emergent Floquet Fermi Surfaces (bottom right).

What are the emergent Floquet Fermi surfaces? Consider a system of fermions driven by a monochromatic electric field with frequency ω. For simplicity, imagine that the fermions move in a crystal with a single Bloch band, and therefore that we have a single Floquet Bloch band with Floquet dispersion $\epsilon(k)$ as a function of crystal momentum k. Imagine also that these fermions are coupled to an ideal heat bath like those considered in Refs. [1–3]. Under these settings, it is possible to show these fermions will approach a unique oscillating many-body steady at late times. Namely, after some time the fermions will lose the memory of their initial conditions and approach a unique state that oscillates with the same frequency ω of the driving electric field. How many fermions occupy in average each of the crystal momenta k in this Floquet-open-system? In equilibrium the answer to this question would be simply that the occupation is given by the standard Fermi-Dirac distribution:

$$n_0(\epsilon_0(k)) = \frac{1}{e^{(\epsilon_0(k)-\mu)/k_B T}+1} \quad (1)$$

Where $\epsilon_0(k)$ is be the standard band energy dispersion. However, the above answer cannot be simply transferred to the Floquet-open-system setting, e.g., by naively replacing the equilibrium band energy $\epsilon_0(k)$ with the Floquet band energy $\epsilon(k)$. We found a remarkable answers [1–3] to this question. First, in the case when the fermions are coupled to an ideal fermionic bath with which they exchange particles and energy by tunneling, the occupation is given by:

$$n(k) = \sum_{l=-\infty}^{\infty} W_l(k) n_0(\epsilon(k) - l\hbar\omega) \quad (2)$$

Here l is an integer that labels the set of functions $W_l(k)$, which are positive weight-like functions that can be explicitly computed from the Floquet band structure (see Refs. [1, 2] for details). This non-equilibrium occupation is illustrated in Fig. 1(a). Interestingly, we see from Eq.(3) that at low temperatures $n(k)$ has a stair-case shape with several steps located at the chemical potential shifted by integer multiples of the driving frequency (black Fig. 1(a)), in sharp contrast to the equilibrium Fermi-Dirac distribution which has a single step at the chemical potential (Fig. 1(a)). At low temperatures these steps evolve into several sharp discontinuous jumps, and the system develops a multiplicity of emergent sharp Floquet-Fermi-surfaces (FFSs), which are defined as the surfaces where the occupation jumps. These FFSs are enclosed inside each other.

Emergent Floquet Non-Fermi liquid state We have also found a remarkable answer for the steady state of periodically driven fermions coupled to bosonic baths in Ref. [3]. Namely, the steady state occupation has a series of non-analyticities at certain momenta, like kinks (Fig. 1(b)), that resemble the Fermi surfaces of a non-Fermi liquid state [3]. Moreover, amazingly, these non-analyticities remain sharp even when the bath is at finite temperature [3]. This is a remarkable finding that has no analogue in equilibrium Fermi liquid states, and leads to the amazing observation that in a sense the Floquet Fermi fluid retains certain quantum properties at finite temperatures that would be washed out by thermal smearing in the usual equilibrium Fermi fluid. For example, due to the sharpness of these non-analyticities, density correlation functions retain quasi-long-ranged power-law and oscillatory decay (i.e. Friedel oscillations) at finite temperature [3]. For the case of parabolic fermions coupled with band mass m and coupled to simple bosonic bath [3], the non-Fermi liquid Floquet Fermi surfaces are located at the following momenta (see Fig. 1(b)):

$$\frac{k_l^2}{2m} = l\hbar\omega \quad (3)$$

Here l is a positive integer. These non-analyticities are created by scattering processes that establish the steady state. More specifically, as we showed in Ref. [3], they arise from a combination of the lack of detailed balance and the presence of Floquet umklapp processes, i.e. that energy is only conserved modulo the frequency of the drive in scattering processes. These ingredients lead to the appearance of non-analyticities of the occupation at certain momenta associated with the Floquet umklapp scattering to the bottom of the Floquet band (see Fig1.(b))). Amazingly these non-analyticities remain sharp even at finite temperature (see Fig. 1(b)), which is a phenomenon with no analogue in equilibrium, a phenomenon that we call "ultra-critical". These kink non-analyticities resemble those of a non-Fermi liquid state in equilibrium, and thus we have called this state the "ultra-critical Floquet Non-Fermi liquid".

Outlook for experimental observation of Floquet Fermi liquid steady states Our work illustrates how Floquet steady states can retain intriguing quantum characteristics. Let us summarize the key experimental conditions to realize such true Floquet steady states of electrons in materials. The visibility of Floquet effects is controlled by the amplitude of Floquet harmonics, which scale as $\sim (ev_F|\mathbf{E}|/\hbar\omega^2)^2$, where ω and $|\mathbf{E}|$ are the frequency and the amplitude of the driving oscillating field. Therefore, in the clean limit it is advantageous to have as low frequency as possible, so there is less heating from the continuous irradiation of electrons. But this frequency should also be larger than the inverse electron lifetime. Therefore, one would like to have clean materials (i.e., lifetimes of tens of picoseconds or larger) and apply radiation with frequencies on the order of 100 GHz (i.e. microwaves). We believe there is a rich and promising landscape of true Floquet steady states in clean materials with non-trivial electronic structures, such as graphene.

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2.33 Non-Hermitian Topology of Correlated Electrons

JAN CARL BUDICH

Non-Hermitian topology of Bloch bands. The idea of effectively modeling dissipative phenomena with a non-Hermitian (NH) Hamiltonian has been widely used for decades (see [1] for an overview), where the imaginary parts of generalized energy eigenvalues account for gain and loss, respectively. In parallel, topological states of matter distinguished by global topological properties rather than local order parameters have emerged as a new paradigm in the classification of matter, as is prominently exemplified by topological insulators and superconductors the advent of which has revolutionized the understanding of Bloch bands in crystalline solids [2].

Building upon and combining the above two developments, NH topology of Bloch bands, i.e. the classification and study of topological properties unique to effective NH Bloch Hamiltonians (or band structures) has recently become a broad frontier of active research [3]. The motivation for considering NH Bloch Hamiltonians ranges from modeling the coupling of a system to an external bath causing loss or (especially for optically active media) gain all the way to accounting for intrinsic sources of dissipation such as inter-particle scattering in correlated electron systems. The focus of our present report is on the latter class of systems, i.e. interacting many-body systems in which the finite lifetime of single particle type excitations, also called quasiparticles, are caused by many-body correlations. More specifically, we address the role of band touchings or crossings in the complex quasiparticle dispersion resulting from the retarded single-particle Green's function in correlated electron systems. Importantly, in NH systems degeneracies, as hallmarking the aforementioned band touchings, generically occur in the form of exceptional points (EP), at which the matrix becomes non-diagonalizable and the eigenvectors associated with the degenerate eigenvalue coalesce [4]. In the following, we will discuss two examples of the profound consequences that the latter observation has on the physics of correlated electrons.

Nodal spectral functions from NH topology. In condensed matter physics, topological semimetals characterized by stable nodal points in their Bloch band structure are of great interest, and dissipative effects such as the finite lifetime of quasiparticles provide a new perspective on nodal band structures and their topological stability. In particular, stable EPs are found in two spatial dimensions, while their Hermitian counterpart, known as Weyl points, are robust only in three-dimensional (3D) systems [3]. Hence, the onset of dissipation may stabilize fine-tuned or symmetry-protected nodal points to topologically protected EPs. Previously, EPs themselves have been considered as the NH analog of band (or level) crossings in a wide range of physical settings, including the complex quasiparticle dispersion in correlated electron systems. However, we note that in basic physical observables such as spectral functions $A(k,\omega)$, the most decisive quantity is the real part of the quasiparticle dispersion, whereas the imaginary part mostly determines how sharp or blurred the quasiparticle band appears in a measurement. We thus find it natural to define nodal spectral functions through the occurrence of crossings in the real part of the quasiparticle spectra, rather than requiring full complex degeneracies tantamount to EPs. Along these lines, we have recently explained the generic occurrence and topological stability of nodal spectral functions as a basic consequence of NH topology. Importantly, EPs appear here as the transition points between phases exhibiting protected crossings in the spectral functions and gapped phases. The predicted nodal phases themselves are thus even more abundant than EPs and occur in 1D systems without requiring symmetry or fine tuning. Their topological stability may be understood intuitively in terms of nontrivial braids formed by the quasiparticle bands in the complex energy plane as a function of the lattice momentum k: any nontrivial braid necessitates a crossing in the projection of the real part of the quasiparticle spectra, i.e., entails a nodal spectral function [5] (see Fig. 1 for an illustration). Besides the basic signature of stable gapless modes in $A(k,\omega)$, we have identified both equilibrium and dynamical physical properties that characterize the corresponding NH topological phases more closely.

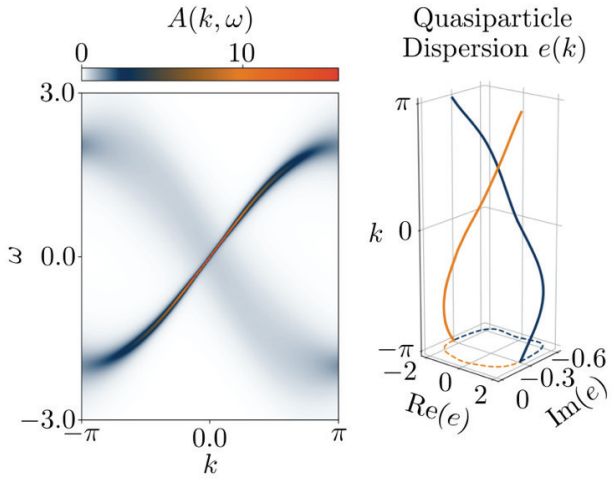

Figure 1: Left panel: Example of a nodal spectral function featuring a gapless almost unidirectional mode. Right panel: Illustration of the associated braiding of quasiparticle bands. Both images are adapted from [5].

From an experimental perspective, the observation of nodal spectral functions and their distinction from gapped systems is conceptually simple, but in practice depends strongly on the ability to tune and resolve the lifetime difference between orbitals or sublattices. The predicted nonreciprocal dynamical effects additionally rely on the ability to selectively excite modes close to nodal points.

Exceptional Luttinger liquids. Luttinger liquid (LL) theory is an important method for describing the low-energy properties of one-dimensional (1D) correlated electrons as an effective bosonic field theory. In higher spatial dimensions, Landau's Fermi liquid theory tells us that the lifetime of quasiparticle excitations generically diverges with temperature as $1/T^2$ when approaching the Fermi surface, thus justifying often an independent particle approximation. By contrast, in 1D, the lifetime $\simeq 1/T$ of single-particle-type electronic excitations defies a free effective description, which may be largely remedied in a range of settings by bosonization that forms the backbone of LL theory. Realistic experimental circumstances to some extent deviate from the ideal zero-temperature fixed point, hence putting finite lifetime effects back on the table in any of the aforementioned scenarios. In addition, whenever scattering rates acquire a nontrivial matrix structure in some orbital or spin degree of freedom, imaginary parts of the excitation spectra may be promoted to intriguing non-Hermitian (NH) topological properties such as EP, the presence of which has an impact on physical properties including transport and dynamics.

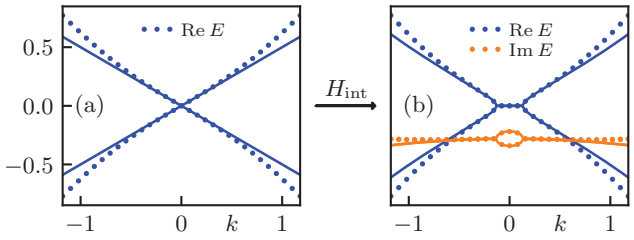

Figure 2: Left panel: Non-interacting dispersion of a generalized SSH model with dots representing the exact dispersion of the lattice model and solid lines the linearized approximation on which the LL analysis is based. Right panel: Upon including sub-lattice dependent interactions, the single particle Green's function acquires a complex spectrum generically replacing the band crossing by an EP structure. Both images are adapted from [5].

In a recent study [6], we have demonstrated how EP structures naturally emerge in LL theory by bosonizing and studying a Hermitian microscopic one-dimensional lattice model of fermions with sublattice-dependent interactions [7]. Upon linearizing the dispersion relation of an extended critical Su-Schrieffer-Heeger (SSH) model (see Fig. 2 left panel), bosonization leads to a novel sine-Gordon-type interaction term of the form $\cos(2\phi(x))\partial_x\phi(x+a)$, where a denotes lattice spacing, and we emphasize that this term is a direct consequence of a sub-lattice dependent interaction strength, which provides the matrix structure of the scattering rates in the sub-lattice degree of freedom, and thus may be seen as the main physical ingredient for the formation of EP structures in our setting. Within this bosonization approach, we have computed the single-particle Green's function at finite temperature by treating the aforementioned interaction term in Matsubara perturbation theory to leading order. Note that in our construction, it has been necessary to keep the lattice spacing finite to obtain rigorous results. This gives rise to an intricate residue structure that we were able to handle by breaking this technically challenging problem down into several manageable parts [6]. Analytic continuation to real frequencies and inference of an effective NH Hamiltonian from the retarded Green's function then yields quasiparticle spectra that feature EP structures (see Fig. 2 right panel) in a wide parameter range respecting the chiral symmetry (CS) of the underlying microscopic lattice model [7]. To corroborate our perturbative analytical findings, we have also provided numerical data based on both the conserving second Born approximation (CSBA) and, for small system sizes, exact diagonalization (ED).

Beyond our present study showing that Luttinger liquid theory is capable of describing EPs, it will be interesting to see which other NH phenomena, such as the NH skin effect, or the anomalous spectral sensitivity of NH systems (see Ref. [3] for an overview) can be captured using the Luttinger liquid framework. Regarding the impact of EP structures on transport properties, an interesting future direction is to study impurity problems, the description of which is one of the main strengths of LL theory, in EP parameter regimes.

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2.34 Advanced Study Group 2019/2022

CONVENOR: PROF. DR. DR. H. C. MULT. PETER HÄNGGI

The objective of this Advanced Study Group (ASG) has been aimed at exploring the realm of open many-body quantum systems which are taken far out of equilibrium. As objects of studies, these systems are located on the interface of several, currently very active, timely research fields such as the physics of open quantum systems, many-body quantum physics, the role of heat and work within quantum thermodynamics, and, last but not least, computational quantum physics.

Signatures of Dissipative Quantum Chaos: Similar to conventional Quantum Chaos (QC), the notion of Dissipative Quantum Chaos (DQC) has been investigated by use those inherent spectral properties of the corresponding, non-unitary generators for the time evolution. Given this task, a strong need exists in establishing universalities, i.e., figuring out unique spectral features, being typical for those properly defined ensembles of generators.

The task in classifying the universal spectral properties has recently been accomplished by several independent groups. This in turn gave rise to a boost of research activities on the DQC topics. A paper on the notion of an ensemble of random Lindblad operators was published by the group's members in October 2019 [10]. Since then, a number of follow-up works on spectral aspects of random Lindblad operators, containing different types of randomness, have been published. In particular, spectral properties of random Lindbladians, on which some additional constrains were imposed, were studied experimentally on the IBM Quantum Experience platform [9].

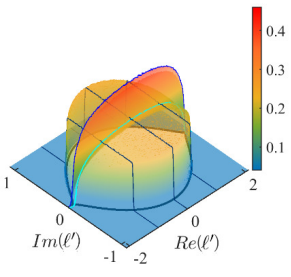

Figure 1: Spectra density of a random Lindbladian (adapted from Ref. [1]).

In own work [1], we generalized the idea of random Lindbaldians further. We presented the concept of super-decoherece, i.e., a decoherence acting on the level of generators of dissipative quantum evolutions. We demonstrated that "superdecoherence" bridges, in a continuous way, Lindblad operators (generators of quantum open evolution) and their classical counterparts, Kolmogorov operators (generators of time-continuous Markovian evolution). We addressed random ensembles of generators, both quantum and classical, evaluated their spectral properties (note Figure 1, depicting the complex-valued spectral distribution of random Linbladians), and demonstrated that the two ensembles are related by superdecoherence. We also defined a procedure of "coherefication" which allows crossing the bridge in the opposite directions, i.e. to obtain a Lindblad operator from a Kolmogorov one. Finally, we addressed the so-called Complex Spacing Ratio measure, which is generalization of a measure used to quantify the degree of chaos in Hamiltonian systems.

In [2] we considered another quantifier of DQC. By unravelling the Lindblad equation describing an open quantum Kerr-nonlinear cavity, periodically modulated in time by coherent pumping of the intracavity photonic mode, into an ensemble of quantum trajectories and employing the recently proposed quantum Lyapunov exponents [8], we identified "chaotic" and "regular" regimes. In particular, we showed that chaotic regimes manifest an intermediate asymptotic power-law in the distribution of photon waiting times. This distribution can be measured explicitly upon monitoring the photon emission with a single-photon detector.

Open Floquet systems: Here we moved along two directions: Are there Floquet Lindbladians? We investigated open quantum systems being subjected to a periodically varying perturbation in time. In other words, the corresponding Hamiltonian is a time-periodic Hermitian operator. The dynamics of such system at weak coupling is governed by a Lindblad equation, possessing a time-periodic generator. – Would it be possible to construct time-independent Lindblad generator (which we termed "Floquet Lindbladian") yielding at stroboscopic instants of times, T, 2T, 3T, ... , the same states of the system as in the case of original time-dependent generator? The answer is always a "yes" in the Hamiltonian limit; this is, however, no longer so when the system is open. In fact, as we demonstrated [3] with a simple driven qubit model, the Floquet Lindbladian does not exist in the most interesting case when the driving is neither diabatic nor adiabatic.

With our consecutive work [4] we advanced further along this line and explicitly demonstrated that different high-frequency expansions, used in recent works as a tool to construct effective Floquet-Lindbladians are, in fact, ill-suited for this task. Correspondingly, the outcome of the study does not provide a firm basis

in order to judge the existence of an effective stroboscopic generator. Nevertheless, we demonstrated that a proper Floquet Lindbladian can be derived from a high-frequency expansion when treating the problem within a suitably chosen rotating frame.

Spectral characteristics of Dissipative Quantum Chaos in Floquet-Markov systems: Novel universal features emerged together with new concepts, such as the "Complex Spacing Ration". These findings resulted upon investigating the Lindblad framework (as discussed above). However, stationary Lindblad generators do not provide a straightforward way to model the semi-classical chaotic regime; therefore, it is seemingly difficult to relate an open quantum dynamics to a dissipative classical dynamics exhibiting chaotic dynamics.

We next considered another type of generator of dissipative quantum evolution, the so-called Redfield generators, which emerge in the Floquet-Markov theory and in turn allow for a semi-classical transition [5]. We used a quantum version of the driven Duffing oscillator as a model to illustrate spectral properties of Redfield generators. Our two main findings here are the following: First, the notion of a random generator alike can be generalized to those being of Redfield-form. Second, Complex Spacing Ratios (CSR) of the generator exhibits Poisson statistics (typical to integrable Lindblad generators) in the chaotic regime, whereas for the regular regime it yields the horseshoe structure (typical to 'chaotic' Lindbladians). In other words, the behaviour becomes reversed when compared to the case of non-random Lindbladians. We attribute this to the fact that the chaotic behaviour of Floquet-Markov systems are encoded within coherent Floquet states of the corresponding Hamiltonians.

Transport in open many-body systems far from equilibrium: Combinations of many-body effects, openness, and strong deviation from equilibrium can lead to transport regimes, which, however, are not accessible in the near-equilibrium limit. In [5], we explored spin transport in an open XXZ chain with strong interaction strength and we demonstrated that the transport features in this system are significantly suppressed, as the bias of the dissipative driving grows large enough. We also detected the regime of negative differential conductance caused by the formation of two oppositely polarized ferromagnetic domains at the edges of the chain. Thus, we demonstrated that this many-body effect, combined with a non-uniform magnetic field, allows for a high degree of control for the spin current.

Workshop "Openness as a resource": An international workshop, entitled *Openness as a resource: Accessing new quantum states with dissipation* took place during the last term of the ASG at the mpi**pks** from January 31 – February 04, 2022. A full detailed report of this workshop can be found in section 3.3.4.

This workshop has been dated towards the end of the 3-rd term so as to crown the various activities addressed by the ASG. The workshop participants represented three different scientific communities: Researchers working on mathematical aspects of open quantum systems that make use of Lindblad generators, semi-groups, and quantum Monte-Carlo methods, their colleagues from the field of quantum thermodynamics [7]. Additionally, theoreticians and experimentalists dealing with circuit-QED and solid-state based quantum systems have attended as well, including a very few topics that were somewhat off-topic although nevertheless quite inspiring.

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2.35 Advanced Study Group 2024/2025

CONVENOR: PROF. ABBAS ALI SABERI

impact physical systems on various scales. Despite their low probabilities, these events hold immense significance due to their potentially catastrophic consequences, making them critically important from a practical standpoint.

Extreme Value Theory (EVT) provides a robust framework for understanding and modeling extreme events, such as unusually large or small values, in systems of independent and identically distributed (i.i.d.) random variables [1]. Its applications span diverse fields, including disordered systems [3], finance, environmental sciences, and engineering. However, many real-world systems exhibit correlations that challenge the classical assumptions of EVT, since correlations significantly influence the statistical behavior of extremes. Recent advances have shown that while classical EVT principles hold for weakly correlated variables, strongly correlated systems often give rise to novel universality classes with unexpected and remarkable properties.

In this context, Random Matrix Theory (RMT) plays a pivotal role in analyzing strongly correlated systems, particularly in characterizing the statistical behavior of eigenvalues. This framework is highly relevant for understanding extreme fluctuations in a variety of complex systems. For example, the interplay between EVT and RMT becomes evident when investigating the limiting distribution and the large deviation probabilities of the largest eigenvalue, with applications to climatic variables in correlated environments. Similarly, fluctuating interfaces within the Kardar–Parisi–Zhang (KPZ) universality classes offer rich examples of strongly correlated systems where extreme events are central.

Building on these foundations, this work explores a range of intriguing phenomena: directed polymers in disordered media, where extreme fluctuations dominate the energy landscape; climatic variables analyzed through the lens of RMT, shedding light on their correlated extremes; variations in percolation thresholds using logistic maps; and the multifractality of wave functions at the critical integer quantum Hall effect (IQHE), where the interplay of EVT and multifractality highlights critical scaling behaviors. These examples demonstrate the rich and diverse applications of EVT and RMT in understanding the extremes and correlations of complex systems, setting the stage for the detailed results presented in the following sections.

Key Outcomes and Research in Progress In our recent work [2], we studied interaction-correlated ensembles of random matrices, where the matrix entries are governed by the Boltzmann measure of a two-dimensional system in thermal equilibrium. The energy function of the system and the temperature define the probability measure, controlling the nature and strength of the interaction. This framework allowed us to investigate how interactions and long-/short-range correlations influence the statistical properties of the eigenvalue spectrum. Our key findings reveal that: (1) at criticality, the eigenvalue spectrum transitions to a universal bell-shaped bulk distribution with a heavy tail, replacing the semicircle law observed off-criticality; (2) extreme eigenvalues at criticality are described by a universal Fréchet distribution, contrasting with the typical Tracy-Widom statistics in standard RMT; (3) in the mean field limit, the spectrum aligns with classical RMT; and (4) the rescaled average extreme eigenvalue emerges as an order parameter, encoding both universal and nonuniversal aspects of the interaction structure. These results underscore the profound impact of criticality and interactions on the universal properties of random matrices.

In an ongoing research (in collaboration with Mehran Kardar (MIT) and Roderich Moessner), we investigated the statistical properties of directed polymers in random media (DPRM) using a six-vertex model framework, mapping to configurations of noncrossing directed paths in a random energy landscape. By expressing the partition function as a product of random transfer matrices, we focus on the largest eigenvalue, which encodes the system's free energy and its fluctuations. Examining its scaling properties over time reveals the same scaling behavior as described by the KPZ equation. Key questions on the agenda include the transition between edge and bulk behavior in the eigenvalue spectrum, the "particle-hole" symmetry between the smallest and largest logarithms of eigenvalues, and whether the arrangement of these logarithmic eigenvalues exhibits hyperuniformity. These investigations aim to deepen our understanding of the connections between DPRM, RMT, and the universal properties of disordered systems.

In collaboration with Jürgen Kurths, Constantino Tsallis, Holger Kantz, and Fatemeh Aghaei, we explore the mapping of percolation models with triadic interaction dynamics onto the logistic map. Our work demonstrates that a variety of complex models, defined on different network structures, can be effectively reduced to the dynamics of the logistic map. This mapping is supported by both numerical simulations and exact analytical derivations, providing a unified framework to study percolation and interaction dynamics within complex systems. This approach offers new insights into the underlying universality and scalability of such systems, with implications for broader applications in

statistical physics and network theory.

In a parallel research (in collaboration with Jürgen Kurths), we extended our methodology to analyze large-scale atmospheric variables using 42 years of ERA5 climate data at 14 atmospheric levels (100–1000 hPa) and CMIP projections up to 2100. Focusing on the spectral properties of key variables, such as the U- (west-to-east) and V- (south-to-north) wind components, we uncovered universal scaling laws in the eigenvalue spectra, indicating long-range correlations and significant deviations from standard RMT predictions. These findings provide crucial insights into the formation of extreme climate events and the effects of anthropogenic warming, emphasizing the potential of this approach to bridge fundamental physics with climate science.

We are conducting research (in collaboration with Martin Zirnbauer) on the multifractality of critical wave functions at the plateau transition of the IQHE, focusing on uncovering their universal properties. Combining theoretical frameworks with extensive simulations, this study addresses longstanding controversies in the field, particularly regarding the spectral properties and scaling behavior of these states. The IQHE provides a pivotal context, characterized by rich multifractal fluctuations and critical exponents that govern the transition between Hall conductance plateaus. By deepening our understanding of critical wave functions, this work seeks to resolve key questions in Anderson localization and shed light on the universal properties of disordered quantum systems at criticality.

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Chapter 3

Details and Data

3.1 PhD Training

The training of PhD students is one of the central tasks of mpi**pks**. It is realized through a large PhD program, our leading role in the IMPRS *Quantum Dynamics and Control* (see next section) and our participation in the IMPRS *Cell, Developmental and Systems Biology* which is coordinated by the Max Planck Institute of Molecular Cell Biology and Genetics.

Prospective PhD students have several options of contacting scientific advisors at the mpi**pks**: PhD positions funded through external grants are advertised in scientific journals and on the internet pages of the institute. Applications for PhD positions funded through the Visitors Program are accepted at all times and invited via the internet pages of the institute, workshop announcements, and print publications.

In 2021, a total of 111 PhD students were working at the mpi**pks**, which includes 91 students from abroad (also counting those who finished or started their studies during that year). The respective numbers for 2022 were 120 PhD students working at the mpi**pks** (94 from abroad), for 2023, 100 PhD students (83 from abroad), and in 2024 we had 90 PhD students (76 from abroad). The overall number of PhD students at the institute at any given time fluctuates between 100 and 120, but the percentage of international students has remained at around 80%. We counted 11 successful final PhD defenses in the year 2022, 15 in the year 2023, and 11 in the year 2024.

In addition to the scientific training by their supervisors, PhD students at the mpi**pks** benefit from a variety of opportunities to develop their expertise, skills, and careers: The students are admitted to the lecture courses offered by the TU Dresden and the mpi**pks** (p. 180). Presentation skills can be practised in regular group seminars or through active participation in the events of the Workshop and Seminar Program. The institute organizes training and career coaching events ranging from a seminar for scientific writing to invited talks by alumni, who provide first-hand information about possible career opportunities (p. 181). Students from foreign countries receive financial and logistic support for joining German language courses.

The majority of the PhD students at the mpi**pks** receive their degree from the TU Dresden (p. 182). After graduation, most continue their research and move to postdoc positions at research institutions all over the world. A smaller fraction takes up non-academic positions in applied research, computer science, finance, or consulting.

3.2 International Max Planck Research School

For a history, participating organizations, and supervisors, see p.13.

PhD students There are currently 52 students enrolled in the graduate school. As befits an international research school, the breakdown of the student body by country of origin shows a large spread: there are 3 students from the Americas (1 from Argentina and 2 from Ecuador), 9 from India, 2 from China and one each from Israel, Japan, Russia, Thailand and Vietnam. The rest are from across Europe

(Czech Republic 10, France 1, Germany 8, Great Britain 2, Greece 2, Italy 1, Poland 2, Serbia 1, Slovakia 2, Spain 3, Sweden 1). Six of the students are women. These students are distributed across the partner institutions: 20 at mpi**pks**, 7 at the Technical University of Dresden, 1 at the Leibniz Institute for Solid State and Materials Research Dresden, 8 at the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, 7 at the University of Chemistry and Technology in Prague, 3 at the University of Wrocław, 1 at the Institute of Low Temperature and Structure Research, 3 at Charles University, 1 at the Wrocław University of Science and Technology (formerly at mpi**pks**), and 1 at the University of Regensburg (collaboration the group of Dr. Marín Bukov at mpi**pks**).

Annual Events The IMPRS organizes various meetings for the students of the graduate school. These meetings take place yearly and they include a retreat that takes place in Germany and a summer school that rotates between Germany, Czech Republic, and Poland. The retreat is typically a three-day meeting framed around student talks and discussions that is partly intended to introduce new students to the activities of the school. This opportunity allows the students to communicate their research to others working in adjacent areas of the physical sciences. The summer school is themed around topics of considerable contemporary interest within the general areas covered by the graduate school.

After several postponements due to the COVID-19 pandemic, the 2022 summer school took place from August 29th to 31st at the conference venue of the Max Planck Society HARNACK HAUS in Berlin, Germany. The event was supported by the Max Planck Society with a EUR 12000 funding. The summer school covered diverse topics including quantum simulation and machine learning.

In 2023 the summer school took place from July 24th to 26th at the Vila Lanna in Prague. In particular, the theme of the summer school was "Light-matter interactions: from atoms and molecules to solids" which has overlaps with the areas of atomic, molecular, and optical physics, condensed matter, and physical chemistry. In a series of 12 lectures a diverse set of topics was covered. These included cavity quantum electrodynamics, photochemistry of molecules, and photoionization by ultrashort pulses. Later that year, from October 4th to 6th, the annual retreat took place in Saxon Switzerland at the Parkhotel Bad Schandau.

The 2024 summer school was organized in the city of Wrocław from July 29th to 31st. A series of 14 lectures was hosted jointly at the University of Wrocław and the Institute of Low Temperature and Structure Research. The topics of the school revolved around machine learning and neural network techniques and their application to many-body systems in/out of equilllibrium. At the beginning of the winter semester, the retreat was organized in Meißen (Germany) from September 30th to October 2nd. Apart from the usual schedule, in this event a short series of soft skills talks was provided to the students in order to strengthen their personal and interpersonal abilities on communications, teamwork, and adaptability.

Other Events The day-to-day operation of the IMPRS is structured around events that offer a forum for the students to meet and discuss. The regular IMPRS seminar is the main vehicle for students and partners of the graduate school to hear about the research activities of the affiliated groups. These seminars feature a colloquium talk given by an external invited speaker and a specialized talk given by an IMPRS student. Both talks have a strong research overlap and conceptually the colloquium introduces the broader context of the research carried out by the IMPRS student. Every IMPRS student gives such a seminar, usually during the final year of the PhD.

The lecture program of the IMPRS is framed around the courses offered by the Technische Universität Dresden during the winter (October–February) and summer (April–July) semesters. The lectures are given by professors at the university and by other members of the various partner institutions, including mpi**pks**. Among the courses offered by the university, the IMPRS selects English language lectures in the topics of the school. Students of the IMPRS are required to complete a certain number of courses monitored by a credit point system.

In addition to the seminar and lecture program, the IMPRS organizes career seminars, in which alumni of the IMPRS are invited back to share their experiences of work and life beyond academia. Our focus in organizing such talks has been on sectors of in which a background in theoretical physics may be attractive to employers, including software engineering and industrial research in machine learning and data science. These talks have proven very popular and are often one of the main ways for students to hear first-hand accounts of career options in which their unique skills and interests have proven valuable beyond academic research.

The day-to-day coordination of the graduate school–contacting students, administration of the applications, advertising, event organization, and the maintenance of the webpage–is carried out by the coordination office at mpi**pks**.

3.3 Workshop and Visitors Program

The Visitors Program of the mpi**pks** hosts guest scientists for a period of up to two years. Excellent working conditions are offered to highly qualified, mostly young, scientists. In close collaboration with the other service departments of the mpi**pks**, the Visitors Program is dedicated to supporting the scientists in every possible way to allow them to focus on their research. This also includes logistic help, e.g., for finding suitable accommodation or obtaining a visa.

A mentoring program and financial support for joining German language courses are in place to make it easy for guests to integrate fast and smoothly into the local community.

International Workshop "Quantum Materials in the Quantum Information Era", September 25 - 29, 2023

During the past years, the numbers of guest scientists including predocs with contracts for at least three months hosted by the mpi**pks** were 271 in 2021, 238 in 2022, 252 in 2023, and 237 in 2024.

In addition to the long-term guest scientist positions, the Visitors Program hosts many short-term visits of up to three months. These visits are usually related to collaborations between the mpi**pks** research groups and other institutes. In this category, the detrimental effect of the COVID-19 pandemic was much more pronounced than for long-term guests, with 2021 bringing a total of only 58 short-term guests. This number increased to 177 in 2022 and only then returned to the pre-pandemic levels of about 300 guests per year, with 270 and 329 guests in 2023 and 2024, respectively.

Guest scientists either join one or more of the in-house research groups or work independently. Alternatively, they may form small temporary groups of their own, working intensely on a particular problem. Many guest scientists actively participate in the Workshop and Seminar Program (see p. 136).

In addition to the regular positions of the Visitors Program, the institute annually offers a Distinguished PKS Postdoctoral Position for experienced postdoctoral scientists. PKS Fellows conduct independent research complementing research areas pursued at the institute and are appointed for three years. Between September 2021 and December 2024, we had six PKS Fellows working at the mpi**pks**: *Dr. Stefano Bo* (until June 2022), *Dr. Nazmi Burak Budanur* (until March 2024), *Dr. Suzy Zhang* (until September 2024), *Dr. Daniel Maria Busiello* (since June 2022), *Dr. Gianluca Teza* (since June 2024), and *Dr. Li Ern Chern* (since October 2024).

To strengthen the transfer of knowledge and experience at the mpi**pks**, the institute annually awards the Martin Gutzwiller Fellowship to a senior scientist who has made exceptional contributions in the area of the physics of complex systems. Gutzwiller Fellows spend up to one academic year at the mpi**pks** and can nominate a young guest scientist for the Visitors Program. Between 2021 and 2024, our institute had the honor to host three Gutzwiller Fellows: *Prof. Benoît Duçot* (Sorbonne University & CNRS), *Prof. Giancarlo Franzese* (University of Barcelona), and *Prof. Siddharth Parameswaran* (University of Oxford), while a visit from *Prof. Silke Biermann* (PSL University) has not been realized yet.

In 2007, the institute launched its first *Advanced Study Group*. These groups consist of 3-5 experienced researchers, who join forces for up to one year to do cutting-edge research on a timely topic from the field of the physics of complex systems. The Advanced Study Group *Open Quantum Systems Far from Equilibrium* under the convenorship of Prof. Peter Hänggi started its work in December 2019, shortly before the global outbreak of COVID-19, and was originally scheduled to be concluded during 2020. As several phases of the intended activities could not be carried out as planned due to travel bans and lockdowns, the Advanced Study Group had to be re-scheduled and finally concluded in 2022. The group *Strongly Correlated Extreme Fluctuations* was convened by Prof. Abbas Saberi in July 2024 and will continue its activities until the end of September 2025 (see reports on p. 47).

A considerable number of guest scientists leave the institute for permanent positions in the academic sector, while many others continue to postdoctoral positions at other institutions in Germany or abroad. Several guest scientists take up positions outside of academia, mainly in sectors such as applied research, informatics, finance, or consulting.

3.3.1 Institute's Fellows

3.3.1.1 Gutzwiller Fellows

Gutzwiller Fellowship 2020/21
(Prof. Benoit Doucot)

Current distribution in Chern insulators. At the beginning of my visit to PKS as a Gutzwiller fellow in 2021, I heard about striking experiments, performed at Cornell by M. Ferguson in K. Nowack's group, on a direct visualization of current patterns in quantum anomalous Hall insulators. Their most remarkable observation is that, against the most common expectations, the non-equilibrium quantized Hall current does not flow along the sample edges, but mostly into wide conduction channels that occupy a significant fraction of the sample bulk [1]. Although surprising, this observation is not in contradiction with established theories. In fact, the well established bulk-edge correspondence states that the quantized Hall conductance in incompressible bulk regions, computed using linear response theory, is the same as the four terminal Hall conductance in the Landauer–Büttiker picture, in which all the non-equilibrium current flows along narrow chiral edge channels. This is an example of what R. Moessner likes to call *topological censorship*: topology by itself fixes only the global response, but does not provide any clue on the details of the spatial current distribution. This distribution is determined by the spatial configurations of the electrochemical and electrostatic potentials inside the sample, which in turn depend on the often complicated interplay between single particle dynamics in a Chern band and Coulomb interactions between electrons.

The authors of Ref. [1] emphasized the apparent similarity of their results with the numerous detailed studies of electrostatic potential profiles across quantum Hall bars in a strong external magnetic field, performed by the von Klitzing group. There, it was found that a large transverse electric field is generated that drives a Hall current across bulk incompressible regions, so that most of the Hall current flows inside these regions. But, together with R. Moessner and D. Kovrizhin, we were led to question this interpretation, after we noted that in the Cornell experiment, Coulomb interactions are very efficiently screened by the top gate, located only 40 nm above the 2D conduction layer. We also noted that the sample geometry probably allows for a finite in-plane component of the electric field generated by the underlying back-gate. As a consequence, electrons in the 2D conducting layer are likely to be subjected to a smooth confining potential, and not just to a sharp one located at the sample boundaries. These considerations led us to consider a new theoretical model for quantum transport in a 2D Chern band, in the presence of this confining potential, and also with relatively strong disorder. As already mentioned,

we assumed that Coulomb interactions do not play a major role in the actual samples. We also assumed that inelastic processes, leading to bulk dissipation, are negligible. This is probably the most questionable hypothesis in our treatment, and one of the interesting directions for future work.

These features of the model define a non-interacting electron problem in a four-terminal scattering geometry, for which the Landauer–Büttiker approach is naturally suited. We have performed extensive numerical calculations using the KWANT package. Because of the large system sizes required for the simulations, we had to use a large number of servers with large amounts of memory, which was only possible because of the excellent computer cluster at **mpipks**and the fantastic technical support provided in-house. They produced a picture (of which an example is given in Fig. 1), according to which most of the current is carried inside wide *compressible* meandering conduction channels that extend over large portions of the system bulk. As can be seen in this figure, the variation of the shape of these channels with the back-gate potential shows a rather good agreement with experimental results.

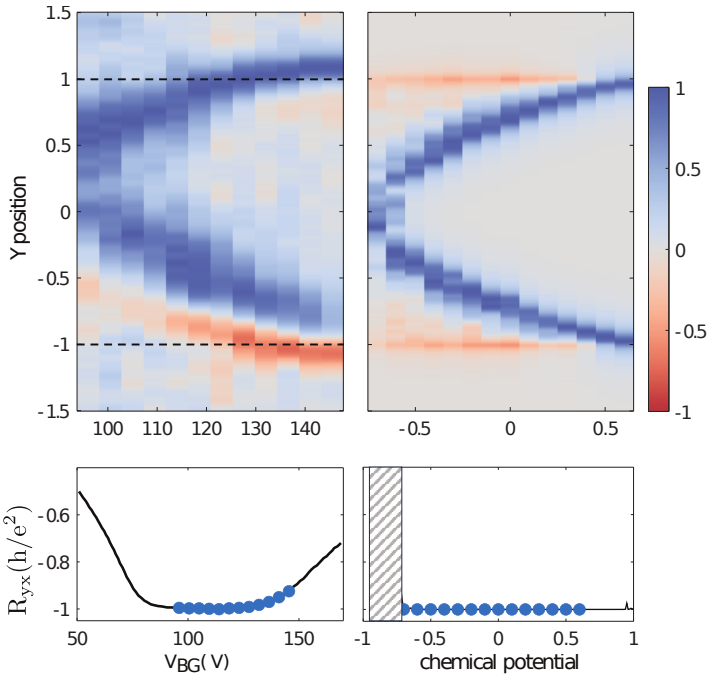

Figure 1: Experiment-theory comparison of the current density distribution in the Quantum Anomalous Hall Effect (QAHE). Left: experiment [1], right: our theory [2]. Top panels show a false colour plot of the normalised current across the sample, vertical axis, against the range of backgate voltages (experiment), or chemical potential (our theory). We only show data where the current is well-quantized, as indicated by the blue points in the bottom panels; quantization breaks down chaotically in the shaded area. At each voltage/chemical potential, we normalize the density by the maximum of its absolute value. The vertical axis is rescaled by the half-width of the system, so that the physical sample boundaries correspond to ± 1, indicated with dashed lines.

On the theoretical side, these *compressible* conduction channels can easily be understood in the absence of disorder. The presence of a transverse electric field E localizes electronic wave-functions along strips, the width of which is given by W/eE , where W is the energy band-width. This spatial scale is usually much larger than the nanoscale that is typical for topological chiral edge states. In the absence of disorder, these strips host a finite number N_{R} (resp. N_{L}) of right (resp. left) moving effective 1D conduction channels. The difference $N_{\mathrm{R}} - N_{\mathrm{L}}$ is equal to the Chern number of the band, so there is an intrinsic chirality in the system. In physical terms, this leads to finite equilibrium currents in the system because of the anomalous velocity affecting electron motion in a Chern band in the presence of a finite electric field. However, in order to reach a sharp quantization of the four-terminal Hall conductance, we need disorder, in order to eliminate (via Anderson localization) all the counter-propagating conduction channels. Our numerical results confirm this scenario, showing a quantum Hall conductance plateau only above a sizable amount of local disorder. We have published this work recently [2] and we would like to pursue it by a more complete analysis of statistical properties of these intriguing meandering conduction channels in the presence of disorder, including the determination of the 1D localization length and the detailed study of the local distribution of currents, which seems very broad from the numerics. A main experimental prediction from our work is that, for samples with fewer screened Coulomb interactions, a

significant amount of conduction should also be observed in the bulk incompressible regions between the meandering channels. This could be checked by removing the top gate used in the Cornell experiments.

Magnon dynamics and entanglement patterns in Skyrmion lattices. During my visit as a Gutzwiller fellow, I also met Nilotopal Chakraborty, who had started a PhD thesis under the supervision of M. Heyl and R. Moessner. Since then, we have started a very fruitful collaboration on several aspects of Skyrmion physics in two-dimensional quantum ferromagnets. This collaboration has led to two published papers [3, 4], including one PRL, and one presently submitted [5].

Magnon dynamics. Motivated by beautiful recent magnon scattering experiments in quantum Hall ferromagnets pioneered at Harvard around 2018, Nilotpal first decided to compute magnon scattering amplitudes across a Skyrmion crystal slab in a 2D quantum Hall ferromagnet. This was quite demanding, both on the conceptual side and then on the computational one. Regarding the former, it was not at all clear to me, at the beginning, how to extend our analytical ansatz for optimal Skyrmion lattices (in the sense that they minimize the repulsive Coulomb energy between individual Skyrmions), developed in earlier works with R. Moessner and D. Kovrizhin, to the case of a spatially inhomogeneous system, in which a slab of a Skyrmion crystal is smoothly connected to semi-infinite ferromagnetic regions on both sides. On the computational side, it transpired quickly that the transfer matrix approach that I had first suggested was ill-behaved numerically, because of the presence of exponentially growing solutions to the linearized equations of motion associated to evanescent modes. For the former problem, I proposed an ansatz to describe the desired inhomogeneous ferromagnet-Skyrmion crystal-ferromagnet configuration, which Nilotpal managed to validate very quickly through numerical calculations. To overcome the numerical instability problem, Nilotpal decided to implement a method developed by J. Pendry to treat light scattering across multi-layered optical media. This allowed Nilotpal to confirm that the striking dichotomy of the magnon spectrum, composed of a collection of effective Landau levels (appearing because of the global twisting spin pattern inside the Skyrmion crystal) at high energy, and a set of gapless Goldstone modes at low energy, could well be evidenced via magnon scattering experiments [3]. In the spring of 2023, he came to visit me, and we arranged a discussion with Preden Roulleau in Saclay, who is one of the experts on magnon scattering experiments in quantum Hall ferromagnets. His response to Nilotpal's presentation of his results was quite enthusiastic, and he decided to design a new experiment to test our predictions. We hope to hear about the results of these experiments soon.

Entanglement patterns. After this, Nilotpal moved to a second project, dealing with a thorough analysis of spatial entanglement patterns between spin and valley pseudo-spin in a graphene layer. A very detailed classification of possible Skyrmion types had been obtained by Yunlong Lian and M. Goerbig in 2017. They showed that, depending on the relative strength of various anisotropic couplings, such as the Zeeman coupling for the spin sector and a uniaxial on-site anisotropy term for the valley pseudo-spin, a single Skyrmion may either involve the spin, the pseudo-spin, or their mutual entanglement degrees of freedom. As for the first two, this latter degree of freedom can also be described in terms of a unit vector on a sphere. Nilotpal was curious to investigate what would happen in a planar system with a finite density of such Skyrmions. For this, we worked in the limit in which the leading term in the effective energy functional is the Coulomb energy between electric charges bound to Skyrmions, because we know exactly how to minimize this energy for periodic configurations in a variational space of holomorphic functions. Assuming that the filling factor of the central Landau level is close to 1, the relevant target space is the complex projective space $\mathbb{C}$P(3), to account for the four internal states available for an electron placed in a given orbital in the central Landau level. In absence of anisotropy, this minimization spontaneously breaks the underlying SU(4) symmetry, giving rise to a degenerate ground-state manifold, in one-to-one correspondence with the full SU(4) group. We designed an efficient procedure to minimize the anisotropic corrections to the total energy over this degenerate manifold. Upon varying the relative strength of various anisotropies, Nilotpal has obtained a rich set of possible spatial entanglement patterns, including smectic and stripe phases [4]. This is quite remarkable, given the fact that all these patterns lead to the same periodic profile for the electric or topological charge density. One possibility to evidence them would be again to perform magnon scattering experiments, since we intuitively expect that the dramatic anisotropic nature of these entanglement patterns would be reflected in strongly anisotropic magnon dispersion relations. This has been confirmed by Nilotpal, who managed to generalize his scattering code from the case of a $\mathbb{C}$P(1) target space to the $\mathbb{C}$P(3) case.

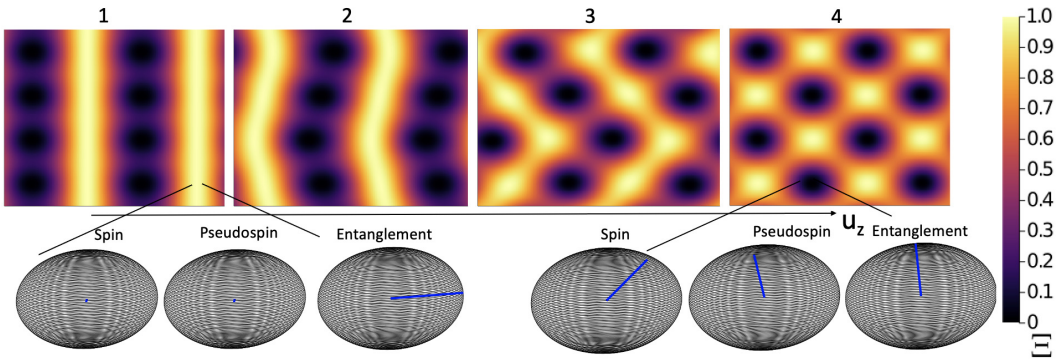

Figure 2: Entanglement patterns of the various entanglement ordered phases obtained on tuning the easy-axis anisotropy coupling constant u_z. Top row: From left to right we see first the formation of continuous straight lines of maximal entanglement $\Xi = 1$ along the y-axis which have a discrete periodicity along x, the *entanglement smectic* (1). Second, these straight lines start to modulate and form wavy patterns with modulated entanglement, which break the continuous translation symmetry of the smectic, while still maintaining a unidirectional nature,the *entanglement stripe* (3). As u_z gets closer to u_p, C_4 symmetry is restored (4). Importantly, the above patterns have the same C_4 symmetric charge density but the entanglement profile breaks C_4 down to C_2. Bottom row: Bloch sphere representation of the local spin, pseudospin, and entanglement vector for maximally (left) and minimally (right) entangled regions.

Entanglemon qubits. In a third project, Nilotpal explored his idea to use the entanglement degree of freedom to design protected qubits. His first intuition was that since the phase β that appears in a Schmidt decomposition of the form $\cos\frac{\alpha}{2}|\phi\rangle + \sin\frac{\alpha}{2}e^{i\beta}|\chi\rangle$, where $|\phi\rangle$ and $|\chi\rangle$ are two orthogonal separable states, does not appear in the expectation values of local spin or pseudo-spin observables, this entanglement phase may lead to more protected qubits than those constructed for example in superconducting circuits, based on the usual U(1) order parameter. We have shown that indeed, it is possible to construct various model Hamiltonians for such *entanglemon qubits*. The simplest family of those exhibits a continuous $\mathrm{U}(1)_\beta$ symmetry, and they are indeed protected (to first order in perturbation theory) to relaxation induced by couplings to the environment via local spin or pseudo-spin operators. To protect them also against dephasing, a possibility is to reduce the continuous $\mathrm{U}(1)_\beta$ symmetry into a discrete Z_2 symmetry. Since we regarded β as a collective variable, this requires to use a certain number of identical copies of basic units composed of a pair of coupled two-level systems (for which entanglement may be defined), and Nilotpal has made some rather concrete proposals on how to implement such design on various physical platforms, including trapped ions, superconducting circuits, quantum dots, and spin-valley $\mathbb{C}$P(3) skyrmions. This work has been written up in the past summer and is now submitted for publication [5].

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[4] N. Chakraborty, R. Moessner, B. Douçot, *Entanglement smectic and stripe order*, arXiv preprint 2312.13362, accepted for publication at Phys. Rev. Lett. (2024).

[5] N. Chakraborty, R. Moessner, B. Douçot, *Entanglemons: Cross-platform protected qubits from entanglement*, arXiv preprint 2409.13019.

Gutzwiller Fellowship 2023/24

(Prof. Giancarlo Franzese)

Overview. I am honored to have received the 2023/24 Martin Gutzwiller Fellowship, allowing me to be part of the **mpipks** research community from November 1, 2023, to April 30, 2024. After my first six-month visit to **mpipks** from November 1, 2022, to April 30, 2023, returning felt familiar and welcoming. I had the opportunity to collaborate with the director, Prof. Frank Jülicher, and a talented member of his group, Dr. Ryota Takaki, along with a new postdoctoral fellow, Dr. Davide Revignas, whom I helped select.

Additionally, to further a collaboration initiated during my previous stay, I continued working with Dr. Ellen M. Adams at the Technische Universität Dresden, affiliated with the Cluster of Excellence Physics of

Life and the Helmholtz Zentrum Dresden Rossendorf. Dr. Adams, an expert in terahertz spectroscopy of interfacial water, and I co-directed a master's thesis during my earlier visit.

During my fellowship, I concentrated on two primary themes. The first was my initial motivation for spending six months with Professor Jülicher, a prominent figure in biomolecular condensation research. I am particularly interested in the role of hydration in the mechanisms that govern liquid-liquid phase separation of biomolecules. Having studied hydration effects at organic and inorganic interfaces for several years, I aim to clarify how incorporating these effects into biomolecular condensation can enhance our understanding of experimental results. Alongside Dr. Adams, we explored the potential impact of small molecule crowders, such as ATP, on the behavior of biomolecular condensates.

The second topic revolves around a research avenue in which I had the privilege to engage with Prof. Jülicher and Dr. Takaki, successfully aligning our mutual interests. This area of investigation focuses on the dynamic evolution of protein adsorption on nanoparticles, which leads to the formation of what is known as the protein corona. During one of the seminars I presented, we discussed this topic and discovered that the glassy behavior I was examining could be effectively described using the Trap model formalism, an area in which both Prof. Jülicher and Dr. Takaki possess extensive expertise.

Finally, the opportunity to concentrate on research allowed me to make significant progress in other projects I was leading. Among these, one of the most notable is the study of the effects of nanoconfinement on fluids and mixtures.

Hydration effects in biomolecular liquid-liquid phase separations. Liquid-liquid phase separation (LLPS) in proteins and nucleic acids is crucial in biology, for example in condensatopathies such as neurodegenerative diseases and cancer. My research focused on understanding the dynamics of LLPS in cellular environments, mainly on how hydration, protein interactions, and biomolecule behaviors affect this process. I also made some preliminary exploration of how the sequences of folded proteins and characteristics of intrinsically disordered proteins influence LLPS. I based my methodologies on my previous studies on fluctuations in liquid-liquid phase transitions. Given that liquid droplets can be metastable states influenced by interactions with cosolutes, I was also interested in investigating these interactions, which are still debated in LLPS literature.

Unstructured proteins play a crucial role in modulating cellular responses to environmental stimuli through processes such as coil-globule transitions and phase separation. Despite their importance, the molecular mechanisms driving these phenomena remain only partially understood. Therefore, during my visit, I published a study in which we employed Monte Carlo simulations based on a coarse-grained (CG) model that considers the effects of water on the free energy of the system [1].

Following previous works, we represented the unstructured protein as a polymer chain. Our primary focus was to explore its response to thermodynamic fluctuations in proximity to a hydrophobic surface. To enhance interactions with the interface, we selected an entirely hydrophobic sequence. Our results revealed that confining the protein within a slit pore lacking top-down symmetry significantly promotes both unfolding and adsorption of the polymer chain, regardless of its state as a random coil or a globule. Additionally, we found that the presence of hydration water influences this behavior, varying with the thermodynamic parameters. These findings offer valuable insights into how homopolymers and unstructured proteins can detect and adapt to external stimuli, such as nanointerfaces or mechanical stresses.

Understanding how hydration water affects free-energy changes in protein solutions requires a molecular perspective. However, biological phenomena often occur at the micron scale, involving numerous biomolecules and millions of water molecules, making atomistic simulations impractical. This complexity has led to the creation of implicit water CG models, which are state-dependent and inadequate for varying thermodynamic conditions. In response, with a Ph.D. thesis that I directed and that was defended during my fellowship, I developed a novel model that allows large-scale explicit water simulations [2]. This model replaces water coordinates with a coarse-grained density field, maintaining critical information about the water hydrogen bond network. By incorporating hydration into free energy calculations, we can gain better insights into protein folding and unfolding behaviors across various temperatures and pressures. This aligns with our previous studies on natural and synthetic proteins and high-concentration aggregation phenomena. Nonetheless, understanding hydration effects within the cellular organization is more complex, and their role within LLPS is still debated.

In collaboration with Dr. Revignas and Prof. Jülicher, we have developed a method to investigate LLPS at moderate protein volume fractions using a CG model that explicitly incorporates contributions from

water. We are currently in the final stages of preparing a manuscript in which we will present detailed calculations. Our conclusions elucidate an entropic mechanism related to the degrees of freedom of water molecules, contributing to the phenomenon of LLPS in protein solutions.

Additionally, in collaboration with Dr. Adams, we investigated the role of adenosine 5'-triphosphate (ATP) in LLPS. Experimental observations indicate that ATP may dissolve condensates, although the mechanism remains unclear. It is hypothesized that changes in water structure are key to the thermodynamics behind this phenomenon. Thus, we explored whether ATP affects the condensates by altering the surrounding water structure. Using terahertz spectroscopy and molecular dynamics simulations, we analyzed the hydration properties of ATP. The simulations identified a hydration shell around the triphosphate group that exchanges water frequently with its environment. Experiments showed changes in the hydrogen bond network around ATP. Our findings suggest that ATP and its counterions can modify water structure. We are currently focusing on whether this disruption in water structure is involved in the ability of ATP to dissolve condensates.

Size-dependent kinetics of nanoparticle protein corona complexes. Nanoparticles (NPs) show promise as efficient drug-delivery systems. Interestingly, biomolecular condensation may also play a role in NP-cell interactions. When introduced into a biological medium, biomolecules adsorb onto the NP, forming a bio-corona that influences the biological behavior of the NP. Experimental evidence suggests that biocondensates facilitate NP uptake through multiple receptor bindings with the bio-corona of the NP, recruiting a microreactor biocondensate for cellular processing. This activity of multi-receptor engagement is contingent on the NP bio-corona and has significant implications for medical applications and therapeutic efficacy. Therefore, engineering the NP bio-corona for efficient drug delivery poses a substantial challenge for nanomedicine. However, understanding how NP characteristics dictate the evolution of this bio-corona over time remains an unresolved issue.

This could be relevant, for example, for designing NPs capable of crossing biological barriers, such as the blood-brain barrier. During my stay in Dresden, I had the opportunity to complete the analysis I began with experimentalists based on synchrotron small-angle X-ray scattering and modeling. We demonstrated that the specific lipid NPs we studied have a barrel-like structure made possible by hydration forces [3].

During my fellowship, I explored the effect of NP size on protein competition kinetics within the corona in partnership with international experimental groups. Through computer simulations and experiments with silica NPs of varying sizes in a blood protein solution, we found that NPs measuring between 40 and 100 nm undergo significant changes in corona composition within 1-30 seconds. Conversely, NPs smaller than 40 nm maintain a stable corona, while those larger than 100 nm evolve slowly over 100 seconds, mirroring behaviors observed in out-of-equilibrium systems. In collaboration with Dr. Takaki, Prof. Jülicher and I examined the time evolution of the corona using the Trap Model, a framework that characterizes glassy dynamics. Our results indicate that the corona stabilization time for NPs exceeding 160 nm may exceed 15 minutes. This highlights the critical influence of NP size on nano-bio interactions relevant for nanomedicine. Furthermore, our findings pave the way for designing advanced drug-delivery vectors for specific time scales by adjusting NP size.

Size–Pore-Dependent Methanol Sequestration from Water-Methanol Mixtures by an Embedded Graphene Slit. The separation of liquid mixtures is crucial for applications like water purification and biofuel production and aligns with the UN Sustainable Development Goals, particularly "Clean Water and Sanitation" and "Affordable and Clean Energy". A promising method involves using graphene slit-pore filters since the confinement impacts the properties of the mixture components, enhancing their separation. However, there has been no systematic study on how pore size affects the thermodynamics of the surrounding mixture.

During the months I spent at the mpi**pks**, I investigated, in collaboration with my group in Barcelona, water-methanol mixtures, using Molecular Dynamics simulations to analyze the effects of graphene pore sizes ranging from 6.5 to 13 Å across three compositions: pure water, 90%-10%, and 75%-25% water-methanol. We discovered that adjusting the pore size alters the pressure, density, and composition of the mixture due to size-dependent methanol sequestration within the pore. Our findings aim to optimize graphene pore sizes for filtration purposes [4].

Industry increasingly demands efficient, sustainable techniques for separating water-alcohol mixtures, with recent advancements in nanotechnology presenting promising solutions. We investigated how the width of a nano-confining graphene slit-pore influences the filtration and purification of water-methanol mixtures.

Our simulations of a coarse-grained model found that specific pore sizes allow for effective segregation of the components, with water preferring the center and methanol clustering near the hydrophobic walls. Furthermore, pore width affects diffusivity non-monotonically, with water diffusing faster than methanol. Therefore, identifying the optimal pore size that capitalizes on segregation and diffusion differences can facilitate the extraction of both components. However, maintaining mechanical stability at specific pore widths requires external forces and work. Our research suggests that a pore size of 12.5 Åmaximizes physical separation while minimizing the energy costs associated with graphene membrane filtration [5].

[1] B. Durà-Faulí, V. Bianco, and G. Franzese, J. Phys. Chem. B **127** (2023) 5541.

[2] L. E. Coronas, and G. Franzese, J. Chem. Phys. **161**, (2024) 164502.

[3] F. Spinozzi, P. Moretti, D. R. Perinelli, G. Corucci, P. Piergiovanni, H. Amenitsch, G. A. Sancini, G. Franzese, and P. Blasi, J. Coll. Interf. Sci. **662** (2024) 446.

[4] R. Bellido-Peralta, F. Leoni, C. Calero, and G. Franzese, Molecules, **28** (2023), 3697.

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Gutzwiller Fellowship 2024

(Prof. Siddharth Parameswaran)

Overview. I had a very productive and stimulating visit to mpi**pks** over 6 months in Spring/Summer 2024. During my stay, I had several interactions with institute members and visitors at all career stages, which has led to many new ideas and to the initiation of new collaborative research projects. During much of my stay, I was accompanied by two graduate students from Oxford, who also benefited greatly from exposure to several new ideas, and mentored a visiting undergraduate intern from Caltech. I also participated formally and informally in several mpi**pks** workshops, speaking at three (FBvHS24, TQMSSP24, and the QUANT24 school), as well as in the CT.QMAT conference of the Dresden-Würzburg excellence cluster. Beyond new work generated by interactions at mpi**pks**, I was also able to complete several long-term projects during the Fellowship. I summarize the various research directions below.

Operator Dynamics on Expander Graphs. My student Ollie Breach, Oxford postdoc Benedikt Placke, mpi**pks** Group Leader Pieter Claeys, and I have initiated the study of operator spreading and entanglement dynamics in systems with the "expander" property (a finite surface-to-volume ratio of subsystems). These are typically viewed as living in infinite-dimensional or hyperbolic space and have recently become the focus of interest due to their complex energy landscapes which make them appealing from the point of view of error correction—specifically, in the context of so-called "Quantum Low-Density Parity-Check" (QLDPC) codes. Ollie has learnt several aspects of quantum circuit technology from Pieter and his group members and has applied this to extract several interesting results on the simplest case of tree graphs. We plan to continue this collaboration after my departure, and it looks likely to lead to at least a few publications. Delving into these sorts of questions was probably the biggest new direction initiated at mpi**pks**. As this had been one of my goals for the sabbatical, this was a very gratifying outcome.

Constrained Dynamics and Response in Topological Phases and Frustrated Magnets. I had several interactions with mpi**pks** graduate student Mark Potts and Roderich Moessner about interesting nonlinear response and constrained dynamics in frustrated magnets such as spin ice, and in topological phases such as Chern bands. This has led to a potential project investigating the interplay of Coulomb interactions and topology in wavepacket dynamics in Chern bands, which may be relevant to future experiments in moiré fractional Chern insulators.

Frustration Graphs and Measurement Dynamics. I had several discussions with mpi**pks** intern Gurkirat Singh (IISc Bangalore) on a range of topics, but most significantly on the role played by "frustration graphs" in influencing measurement-only dynamics (the subject of my TQMSSP24 talk). Remarkably, Gurkirat was able to invent a simple all-to-all toy model that captures much of the basic phenomenology. We intend to continue studying this question as part of his Masters' thesis alongside Benedikt Placke, for which purpose Gurkirat may visit us in Oxford. I also benefited from discussions with several participants of the LOCALI24 workshop which touched on related topics.

Moiré Materials. Among my most active topics of current research are moiré materials—the subject of both my Gutzwiller Colloquium and my talk at FBvHS24. While there are no moiré-focused groups at mpi**pks**, I had several stimulating discussions on the topic with mpi**pks** members and more in-depth interactions with various visitors. I was able to complete a long-running project on "Textured Exciton

Insulators", unusual forms of broken-symmetry states that emerge in topological bands, leading to a pair of preprints. I also completed a joint experiment-theory project with the group of Mitali Banerjee (EPFL), and continued discussions with my group remotely. Some ongoing work on fractional Chern insulators in twisted $MoTe_2$ benefited greatly from discussions with the FBvHS24 participants. Finally, my student Konstantinos Vasiliou accompanied me to **mpipks** during my visit and decided to learn some quantum Monte Carlo (QMC) from **mpipks** staff scientist Johannes Hoffman, which appears likely to lead to a new collaboration studying textured exciton states using QMC.

Spin Liquids on the Trillium Lattice. While at **mpipks** I also completed a long-running project on parton-mean field theory of spin-1/2 quantum spin liquids on the three-dimensional trillium lattice of corner sharing triangles. Fortuitously, Yasi Iqbal (IIT Madras) was visiting to speak at TQMSSP24, and was working on the same problem from a different direction. Beyond some very useful feedback on our work, Yasir suggested that our groups join forces to tackle the more experimentally relevant spin-1 case, leading to another new collaboration.

Charge Pumps and Unnecessary Criticality. While at **mpipks**, I initiated work that was stimulated in part by discussions on a flurry of work on "Higher Berry Phases"; in the course of various conversations, I realized there was a connection to older work involving my Oxford postdoc Abhishodh Prakash. We were able to explain how a seemingly unnecessary critical surface in a simple one-dimensional model we had studied a couple of years ago could be explained in terms of a topological "pumping" property of the sequence of gapped phases that encircle the critical surface. The work benefited from conversations with several **mpipks** members, notably Gurkirat Singh and Chris Hooley.

Variational Approaches to SYK Problems. I worked with a **mpipks** intern from Caltech, Amir Ibrahim, on variational approaches to understanding ground states of Sachdev–Ye–Kitaev-like problems. Although the problem hit a stumbling block in the form of a relatively little-known paper that showed that the naïve variational principle (Hartree–Fock) is not satisfactory in this setting, it nevertheless was an excellent learning experience for Amir and raised several interesting questions that we hope to pursue in the future.

3.3.1.2 PKS Fellows

Distinguished PKS Postdoctoral Fellowship 2021-2024
(Shu Zhang)

My research activities have been both explorative and productive during the stay at **mpipks** from 2021 to 2024. Centered around the theme of magnetic dynamics and transport, I have worked on diverse topics including frustrated magnetism, topological magnons, open-system spin dynamics, and quantum-impurity relaxometry. The vibrant scientific environment at **mpipks** has provided me with the opportunities to engage in collaborations not only with internal members, but also with researchers across the Dresden area and internationally. I summarize the main research findings below.

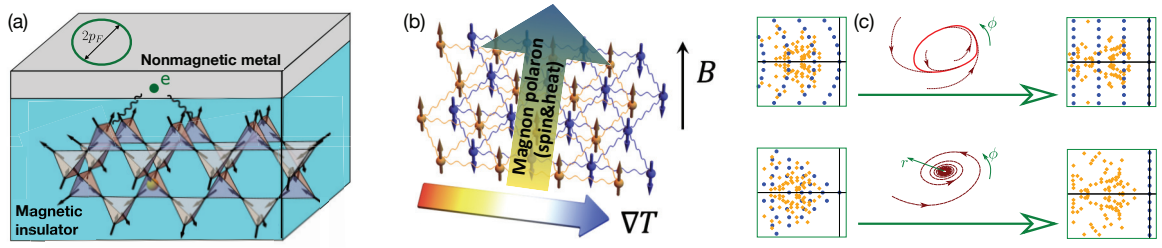

Figure 1: (a) A heterostructure of a nonmagnetic metal thin film on a bulk magnetic insulator. The proximitized anomalous transport arises as the itinerant electrons from the metal are scattered by the localized magnetic moments in the magnet. (b) A bilayer of van der Waals magnets with an intralayer ferromagnetic interaction and a weak interlayer antiferromagnetic interaction. Topological magnon polarons in the system can give rise to thermal Hall and spin Nernst effects. (c) The fate of Liouvillian spectra (left) in approaching the classical limit (right). For a limit cycle (top) the signature is a branch of equally spaced imaginary eigenvalues, and at a Hopf bifurcation point (bottom) the spectrum collapses onto the imaginary axis.

Anomalous transport in proximity to complex magnetic insulators. Low-energy spin fluctuations play an important role in the dynamical and transport behavior of complex magnetic insulators, but are often challenging to probe directly with the current experimental techniques. We suggest a possible probe of spin fluctuations with proximitized transport in a nonmagnetic metal/magnetic insulator heterostructure, in which the itinerant electrons from the metal are scattered by the localized magnetic moments in the magnet [Fig.1(a)]. In collaboration with an experimental group, we have studied a heterostructure of the metallic pyrochlore $Bi_2Ir_2O_7$ and the pyrochlore quantum magnet $Yb_2Ti_2O_7$ [1]. The scaling behavior of the resistance of the metal as a function of the temperature and the magnetic field can be related to the dynamic spin-correlation functions of the magnet, which serves as strong evidence for proximity effects. Our theoretical modeling based on a Boltzmann-equation approach, taking into account the short-range spin fluctuations in $Yb_2Ti_2O_7$ can explain very well the counterintuitive scaling of the proximitized magnetoresistivity. These findings demonstrate a pathway for coupling quantum spin degrees of freedom to itinerant electrons, offering new possibilities for functional quantum materials and applications in spintronics.

Topological Magnon-Polaron Transport. Topological magnons have gained much attention as they can lead to transverse channels for heat and spin transport, promising for spintronic and heat-management applications. Recently, my coauthors and I have pointed out that magnon-phonon hybridization can provide a generic mechanism to support spin-carrying topological bosonic modes. Together with a summer intern at mpi**pks**, we have studied an antiferromagnetic van der Waals bilayer with couplings between magnons and elastic degrees of freedom. We find the magnon-polaron excitations to be topologically nontrivial [2], and show that they can lead to thermal Hall and spin Nernst effects [Fig.1(b)]. The bilayer system features a topological transition associated with the metamagnetic phase transition. As a result, the thermal Hall conductance undergoes a sign change. An analysis of Berry curvature reveals distinct topological structures in the antiparallel and parallel magnetic phases, further elucidating the underlying mechanisms and underscoring the potential of van der Waals magnets for tunable topological transport effects.

Open-system spin dynamics and transport. A more recent direction of my research focuses on bridging the semiclassical methods typically used in spintronics and the open-quantum-system methods in quantum optics to treat driven dissipative spin dynamics. Together with other researchers at mpi**pks**, I have investigated a spin model governed by a Markovian master equation, and revealed the quantum spectral features corresponding to the emergence of coherent limit-cycle oscillations and algebraic decay in the classical (large-spin) limit [3]. Limit cycles are characterized by slowly-decaying branches with vanishing decoherence rates in the Liouvillian spectrum, while power-law decay at a Hopf bifurcation is associated with a spectral collapse [Fig.1(c)]. Such features turn out to be generic, which we also demonstrate with a lossy Bose–Hubbard dimer, and provide a resolution to the apparent contradiction between the exponential decay expected from a gapped Liouvillian spectrum and the persistent classical oscillatory dynamics. Our insights provide a broader understanding of quantum-classical correspondence in dissipative systems and establish a foundation for further exploration of nonlinear quantum dynamics.

In collaboration with external researchers,I have explored analogies of spintronic platforms to atoms in a cavity. An analogy can be based on a bare-bones model with two species of spins interacting via a long-wavelength boson in which one species of spins undergoes incoherent pumping. This model gives rise to an interplay of lasing and superradiance [4], predicting the possibility of a magnon lasing transition in a spintronic device with strongly broken U(1) symmetry. We have also contributed to the study of the non-Hermitian skin effect (NHSE) in open magnetic systems and the resulting transport properties. In this work [5], we establish a link between the dynamics governed by the non-Hermitian Hamiltonian with those of the full Liouvillian, as well as with classical magnetization dynamics.

Quantum-impurity relaxometry to reveal magnetic dynamics. Quantum sensing techniques utilizing nitrogen-vacancy (NV) centers in diamonds are particularly useful to investigate magnetic phase transitions and spin fluctuations at the nanoscale. I have collaborated with an experimental group in a series of works on NV relaxometry, for example, to reveal the domain formation and spin fluctuation behaviors in a topological material, $MnBi_2Te_4$ [6]. Furthermore, engineered magnetic domain walls have been used to locally control NV centers, opening new pathways for hybrid quantum spintronic devices [7]. My ongoing work together with a Ph.D. student at mpi**pks** theoretically predicts the relaxometry features of the magnetic Berezinskii–Kosterlitz–Thouless transition, which can inspire further experimental study of topological phase transitions.

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Distinguished PKS Postdoctoral Fellowship 2022-2025

(Daniel Maria Busiello)

Overview. During my stay at mpi**pks**, I worked on several topics ranging from biochemical systems to information processing. The idea behind my research activity has always been to understand the intimate connection between observed emergent behaviors and microscopic determinants underpinning their onset. This general question has been tackled from different perspectives, employing tools of stochastic thermodynamics and information theory. Here, I present a brief description of the main outcomes stemming from my research stay at mpi**pks**, obtained both in collaborations with institute members and external collaborators.

Thermodynamically accessible space for chemical systems. I performed this work in collaboration with Shiling Liang, PhD student at EPFL under my supervision at that time and currently at mpi**pks**, and Paolo De Los Rios (EPFL). Biological and living systems continuously harvest and consume energy to perform their tasks, therefore working out of equilibrium. Moreover, they usually operate with a limited energy budget which imposes crucial constraints on their biological functioning. In this work [1], we focus on a specific feature of chemical systems, namely their ability to select desired chemical states through dissipation-driven mechanisms. These selection phenomena are ubiquitous, from DNA replication to cellular signaling and pattern formation. They rely on continuous energy dissipation into the environment, thereby breaking symmetries holding at equilibrium. We show that any selection process is universally constrained by the total energy budget, independently of the details of the underlying dynamics. In particular, the accessible space of any biochemical system, i.e., the range of concentrations each chemical species can explore, is uniquely determined by the forces pushing it out of equilibrium. First, we derived this thermodynamic space for a simple kinetic proofreading scheme, i.e., a mechanism at the core of accurate genome duplication and protein synthesis, generalizing previous results on its maximal achievable performance. Finally, we studied the formation of spatial patterns of chemical concentrations, a phenomenon gaining increasing interest in biochemical contexts. We find that, once again, the energy budget of the system constrains the possibility of observing these patterns, i.e., their contrast. Our results unveil the intimate connection between energy dissipation and selection phenomena, opening the avenue to understanding how non-equilibrium conditions shape the observed properties of all biochemical systems.

Unraveling active baths from hidden degrees of freedom. In the line of work aiming to understand the role of energy dissipation in establishing robust biological function, in this work [2], done in collaboration with Matteo Ciarchi and Ivan Di Terlizzi, both at mpi**pks**, we investigated the main ingredients to provide a thermodynamically consistent description of active systems, i.e., systems that are maintained away from equilibrium via internal or external energy-consuming processes such as bacteria, enzymes, and proteins. A common situation in experimental and theoretical settings is that these active systems act as an environment for passive probe particles, the dynamics of which is affected by the bath in which they are immersed. Starting from the description of all degrees of freedom (DOFs), both belonging to the bath and the probe particle, we showed that there exist two classes of DOFs, non-entropic and entropic ones. The first ones can be integrated out exactly without affecting the entropy production rate of the whole system, leading to a thermodynamically consistent description of the observed DOF by means of a stochastic equation with memory. By contrast, if one integrates out dissipative DOFs, the entropy production rate changes dramatically, increasing or decreasing, making a thermodynamically consistent description of the probe dynamics impossible. These results shed light on the controversial problem of characterizing the dissipation of probe particles immersed in an active bath without relying on phenomenological descriptions or information-limited modeling.

Information processing in multiscale stochastic systems. Non-equilibrium activity in biological and living systems is key to ensure their robustness. Indeed, these systems have to sense, process, and adapt to a multitude of cues reliably in very dynamic and noisy environments. Establishing accurate processing of this external information is then instrumental to sustain biological functioning and the emergence of large-scale organisation. Biological information processing is often implemented through a series of interconnected fluctuating processes that evolve on a wide range of temporal and spatial scales. Examples range from neural networks to ecological communities or chemical signaling architectures. I explored these information-processing systems in very general terms, elucidating some key aspects underpinning their performance. In a first work [3], done in collaboration with Giorgio Nicoletti, at EPFL at that time, we studied the intimate relationship between the presence of causal couplings between internal processes and their ability to share information effectively. We derived the foundational rules governing information propagation in any multiscale system, independently of its dynamics, highlighting that information can only be generated by slowly-evolving processes, while it can be propagated from fast to slow variables through causal interactions. As such, causality does not necessarily imply shared information when multiple timescales are involved. A second work [4] along this line, again in collaboration with Giorgio Nicoletti, explored the complex scenario in which living systems do not have access to all DOFs. As such, they need to transduce information from these hidden DOFs to operate efficiently. For example, the internal processes of a red blood cell can only access the external world through the cellular membrane: but how well can this membrane transmit such information? And how can information transmission be achieved with a limited energy budget? Our work shows that, by optimizing energy and information at the same time, biological systems can tune themselves to harvest maximal information from the environment. These highly efficient strategies require a price in terms of energy consumption, but this price is far outweighed by the information learned about the hidden, external signals. A particularly relevant case study for our results is red blood cells. We quantify how much information about the state of the internal cytoskeleton is transmitted to the flickering of their membrane, unraveling a deep connection between healthy cellular conditions, energy dissipation, and information. In particular, the mechanical stress of the cell affects its efficiency in terms of how well information is transmitted, providing novel and fundamental insights into the functioning of biological systems in complex environments. This work has also been highlighted in a Viewpoint in Physics Magazine.

Other research directions. My research activity at mpi**pks** explored many other directions. To cite only some examples, I explored the functioning of biochemical transporters [5], the performance of different kinetic proofreading schemes [6], various fundamental problems in stochastic thermodynamics [7, 8], and the functional role of habituation phenomena—the progressive decay of the response upon repeated stimulations—in chemical signaling networks [9]. All these results contributed to the understanding of how biological systems use energy to process information and perform complex tasks efficiently.

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3.3.2 Conferences, Workshops and Symposia

The COVID-19 pandemic still had an impact on the workshop program during the years 2021 and 2022, and a hybrid format was widely used for workshops over this time period. However, over the year 2022 the pandemic situation improved gradually and a return to mostly on-site events was possible. The technical equipment and expertise developed to hold hybrid workshops during the pandemic enabled giving workshop organizers the option of hybrid participation to accept remote applicants as audience participants in workshops. The hybrid system also allows for virtual talks to be held if a contributor is unexpectedly unable to travel, which in the past would have led to their contribution being cancelled.

The plans for binodal workshops at the institute eventually matured into the first event of this kind, the "Flat bands and high-order Van Hove singularities" seminar and workshop in the spring of 2024. Using

the technical setup for hybrid events, it was possible to conduct the workshop simultaneously at two hubs in different continents: mpi**pks** in Germany and the Center for Theoretical Physics of Complex Systems of the Institute for Basic Science in Daejon, South Korea. This format, which is planned to be extended to other collaborating institutions in the future, gives contributors and participants the option to join their local workshop node, which reduces the necessity of intercontinental travel for a short period and reduces the carbon footprint of the workshop.

*List of workshops held at **mpipks** between 01.10.2025 and 31.12.2024*

1. *Ergodicity Breaking and Anomalous Transport in Quantum Many-Body Systems*
   Hybrid Workshop: October 04 - 08, 2021 — 203 participants
   Scientific coordinators: F. Evers, A. Mirlin
2. *Probing Complex Quantum Dynamics through Out-of-Time-Ordered Correlators*
   Hybrid Workshop: October 11 - 15, 2021 — 170 participants
   Scientific coordinators: R. A. Jalabert, K. Richter
3. *Openness as a Resource: Accessing New Quantum States with Dissipation*
   Hybrid Workshop: January 31 - February 04, 2022 — 129 participants
   Scientific coordinators: S. Denisov, M. Campisi, P. Hänggi
4. *Ordinal Methods: Concepts, Applications, New Developments and Challenges*
   Hybrid Workshop: Feburary 28 - March 04, 2022 — 64 participants
   Scientific coordinators: J. M. Amigó, K. Keller, O. Rosso
5. *Physics and Collective Dynamics of Future Mobility*
   Hybrid Focus Workshop: March 09 - 11, 2022 — 56 participants
   Scientific coordinators: M. Barthelemy, C. Sommer, M. Timme
6. *Topological Materials: From Weak to Strong Correlations*
   Focus Workshop: April 11 - 13, 2022 — 142 participants
   Scientific coordinators: S. Bühler-Paschen, T. Neupert, Q. Si
7. *Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers*
   Hybrid Focus Workshop: April 25 - 28, 2022 — 67 participants
   Scientific coordinators: M. Hafezi, F. Pollmann, A. Smith
8. *Emergent Hydrodynamics in Condensed Matter and High-Energy Physics*
   Hybrid Workshop: May 02-06, 2022 — 115 participants
   Scientific coordinators: A. Gromov, D. Son, P. Surowka
9. *Chimera States: From Theory and Experiments to Technology and Living Systems*
   Hybrid Workshop: May 16-20, 2022 — 77 participants
   Scientific coordinators: J. Davidsen, Y. Maistrenko, K. Showalter
10. *Quantum Chaos and Holography*
    Workshop: May 30 - June 03, 2022 — 48 participants
    Scientific coordinators: H. Liu, A. Polkovnikov, M. Rozali
11. *Band Topology in Quantum Magnets: From Nontrivial Excitations to Non-Hermitian Topology and Spintronics*
    Hybrid Focus Workshop: June 13 - 15, 2022 — 89 participants
    Scientific coordinators: P. A. McClarty, J. G. Rau, J. Romhányi
12. *Intelligent Machines? – Self-Organized Nonlinear Dynamics of Machines across Scales*
    Hybrid Workshop: June 20 - 24, 2022 — 54 participants
    Scientific coordinators: N. Hoffmann, P. Manoonpong, M. Timme
13. *Dynamics of Immune Repertoires: Exploration and Translation*
    Hybrid Seminar and Workshop: July 07-30, 2022 — 261 participants
    Scientific coordinators: A. Eugster, U. Hershberg, M. Or-Guil, G. Yaari

14. *New Trends in Nonequilibrium Many-Body Systems: Methods and Concepts*
    Workshop: August 01 - 05, 2022 — 56 participants
    Scientific coordinators: F. Heidrich-Meisner, T. Oka, P. Werner
15. *Shedding Quantum Light on Strongly Correlated Materials*
    Workshop: August 22 - 26, 2022 — 56 participants
    Scientific coordinators: A. Imamoglu, D. Jaksch, F. Piazza
16. *Quantum Transport with Ultracold Atoms*
    Workshop: August 29 - September 02, 2022 — 119 participants
    Scientific coordinators: H. Ott, S. Wimberger
17. *Inverse Network Dynamics - Network Structure and Function from Nonlinear Dynamics and Time Series Data*
    Hybrid Seminar and Workshop: September 12 - 21, 2022 — 100 participants
    Scientific coordinators: K. Lehnertz, M. Nitzan, M. Timme
18. *QED Laser Plasmas*
    Workshop: September 26 - 30, 2022 — 42 participants
    Scientific coordinators: A. Di Piazza, S. Mangles, M. Marklund
19. *From Quantum Matter to Quantum Computers*
    School: October 04 - 07, 2022 — 372 participants
    Scientific coordinators: M. Bukov, P. Claeys, A.-C. Heinrich, R. Moessner
20. *Topology and Non-Equilibrium Dynamics in Engineered Quantum Systems*
    Hybrid Workshop: October 10 - 14, 2022 — 187 participants
    Scientific coordinators: M. Aidelsburger, A. Eckardt, W. Hofstetter
21. *Interdisciplinary Life of Microbes: From Single Cells to Multicellular Aggregates*
    Workshop: November 07 - 11, 2022 — 60 participants
    Scientific coordinators: L. Chai, E. Shank, V. Zaburdaev
22. *Atomic Physics 2022*
    Workshop: November 28 - December 02, 2022 — 70 participants
    Scientific coordinators: J.-M. Rost, M. Eiles, A. Eisfeld
23. *Physical Biology Circle Meeting 2023*
    Focus Workshop: January 30 - February 01, 2023 — 132 participants
    Scientific coordinators: F. Jülicher, P. Haas, S. Rulands
24. *Spring School on Modern Topics in Condensed Matter*
    School: April 17 - 21, 2023 — 48 participants
    Scientific coordinators: A. Mackenzie, R. Moessner
25. *New Perspectives in Active Systems*
    Hybrid Workshop: April 24 - 28, 2023 — 210 participants
    Scientific coordinators: C. Huepe, F. Peruani
26. *Dynamical Control of Quantum Materials*
    Workshop: May 22 - 26, 2023 — 75 participants
    Scientific coordinators: D. Kennes, J. McIver, M. Sentef
27. *Decomposing Multivariate Information in Complex Systems*
    Workshop: June 05 - 09, 2023 — 64 participants
    Scientific coordinators: C. Finn, A. Pakman, M. Wibral
28. *Active Matter at Surfaces and in Complex Environments*
    Workshop: June 19 - 23, 2023 — 83 participants
    Scientific coordinators: M. Tasinkevich, M. Telo da Gama, W. Uspal
29. *Control of Ultrafast (Attosecond and Strong Field) Processes Using Structured Light*
    Seminar and Focus Workshop: June 26 - July 14, 2023 — 66 participants
    Scientific coordinators: C. Hernández-Garcia, M. Ivanov

30. *Elastic Manipulation and Dynamics of Quantum Materials*
    Seminar and Workshop: July 31 - August 11, 2023 — 95 participants
    Scientific coordinators: J. Schmalian, J. Sinova, R. Valenti

31. *Non-Hermitian Topology: from Classical Optics to Quantum Matter*
    Workshop: August 14 - 18, 2023 — 78 participants
    Scientific coordinators: E. J. Bergholtz, F. Piazza, J. C. Budich

32. *Extreme Waves*
    Workshop: August 28 - September 01, 2023 — 56 participants
    Scientific coordinators: N. Akhmediev, H. Brand, A. Chabchoub

33. *Scientific Workshop: 30 years* ***mpipks***
    Workshop: September 06 - 09, 2023 — 83 participants
    Scientific coordinators: F. Jülicher, R. Moessner, J.-M. Rost

34. *Korrelationstage 2023*
    Workshop: Sept 11 - 15, 2023 — 98 participants
    Scientific coordinators: I. Eremin, L. Fritz, M. G. Vergniory

35. *Quantum Dynamics - Fundamentals and Realizations*
    School: September 18 - 22, 2023 — 94 participants
    Scientific coordinators: M. Bukov, P. Claeys, R. Moessner, S. Rockenstein

36. *Quantum Materials in the Quantum Information Era*
    Workshop: September 25 - 29, 2023 — 69 participants
    Scientific coordinators: J. Checkelsky, Q. Si, R. Valenti

37. *Non-autonomous Dynamics in Complex Systems: Theory and Applications to Critical Transitions*
    Seminar and Workshop: October 09 - 27, 2023 — 87 participants
    Scientific coordinators: P. Ashwin, U. Feudel, M. Ghil

38. *Atomic Physics 2023 - with focus days on "Research Highlights in the Eyes of Editors"*
    Workshop: November 27 - December 01, 2023 — 71 participants
    Scientific coordinators: J.-M. Rost, T. Pattard

39. *Quantum thermalization, localization and constrained dynamics with interacting ultracold atoms*
    Focus Workshop: December 06 - 08, 2023 — 27 participants
    Scientific coordinators: F. Heidrich-Meisner, M. Aidelsburger, F. Pollmann

40. *Fractional Quantum Anomalous Hall Effect and Fractional Chern Insulators*
    Workshop: February 05 - 08, 2024 — 78 participants
    Scientific coordinators: Z. Liu, J. van den Brink, Y. Zhang

41. *Quantum Interactive Dynamics*
    Workshop: March 12 - 15, 2024 — 34 participants
    Scientific coordinators: R. Moessner, F. Pollmann, A. Smith, S. Sondhi

42. *Information processing, Noise, and Adaptation in Living Systems*
    Hybrid Workshop: April 15 - 19, 2024 — 66 participants
    Scientific coordinators: N. Barkai, D. M. Busiello, C. Zechner

43. *Interdisciplinary Challenges in Non-Equilibrium Physics: from Soft to Active, Biological and Complex Matter*
    Workshop: April 22 - 26, 2024 — 102 participants
    Scientific coordinators: X. Chen, M. Rinaldin, A. Sciortino

44. *Chemotaxis – from Basic Physics to Biology*
    Hybrid Workshop: May 13 - 17, 2024 — 57 participants
    Scientific coordinators: R. Insall, J. Simmchen

45. *Flat Bands and High-Order Van Hove Singularities*
Seminar and Binodal Workshop: May 27 - June 07, 2024 — 73 participants in Dresden
Scientific coordinators (Dresden): C. Chamon, L. Classen, J. Betouras — 147 participants in total

46. *Geometry and non-adiabatic responses in non-equilibrium systems*
Workshop: June 17 - 21, 2024 — 85 participants
Scientific coordinators: P. W. Claeys, N. Goldman, M. Kolodrubetz

47. *Non-equilibrium Many-body Physics Beyond the Floquet Paradigm*
Workshop: June 24 - 28, 2024 — 96 participants
Scientific coordinators: R. Moessner, G. Refael, H. Zhao

48. *Topological Quantum Matter in Magnetic and Synthetic Platforms*
Workshop: July 08 - 12, 2024 — 62 participants
Scientific coordinators: H. Bernien, R. Samajdar, H. Yan

49. *Chemical Coding at the Atomic Scale: Designing Hybrid and Quantum Nanostructures for Applications in Optical Biosensing, Light Harvesting, Chiral Catalysis, and More*
Hybrid Workshop: August 19 - 23, 2024 — 60 participants
Scientific coordinators: S. Erwin, A. Eychmüller, A. Govorov

50. *Collective Phenomena in Quantum Many-Body Physics: From Quantum Matter to Light*
School: September 09 - 13, 2024 — 59 participants
Scientific coordinators: M. Bukov, P. Claeys, R. Moessner

51. *Localization: Emergent Platforms and Novel Trends*
Hybrid Workshop: September 16 - 20, 2024 — 108 participants
Scientific coordinators: F. Evers, I. A. Gruzberg, A. Mirlin

52. *Matter to Life Fall Days*
Symposium: October 01 - 02, 2024 — 109 participants
Scientific coordinators: J. Heidelberger, D. Madhavan, F. Jülicher

53. *Electronic Correlations and Beyond - in Memory of Peter Fulde*
Workshop: October 03 - 05, 2024 — 68 participants
Scientific coordinators: F. Jülicher, R. Moessner, J.-M. Rost

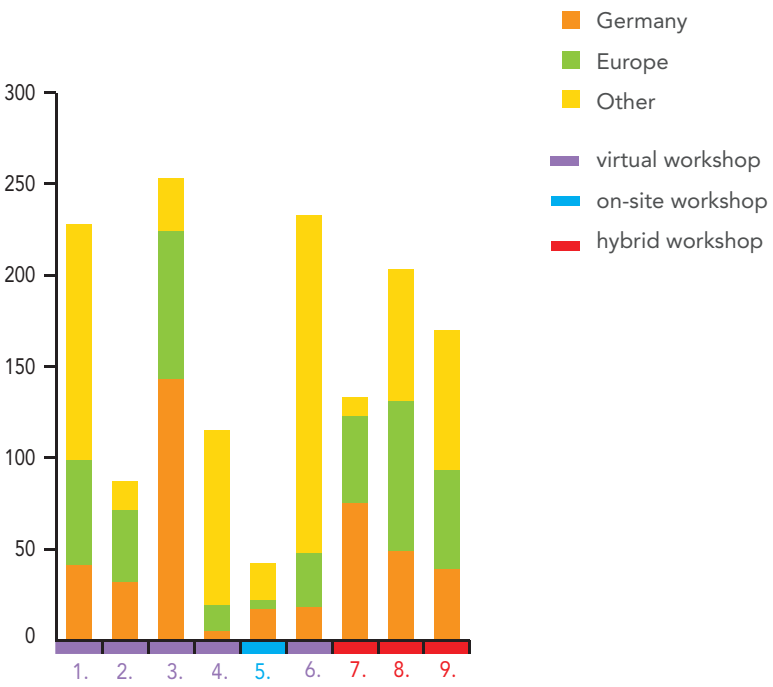
54. *Quantum Meets Classical*
Workshop: October 07 - 11, 2024 — 59 participants
Scientific coordinators: A. Chandran, S. Gopalakrishnan, C. Laumann, V. Oganesyan

55. *Future of Ultracold and Ultrafast Dynamics*
Workshop: October 21 - 25, 2024 — 57 participants
Scientific coordinators: M. Eiles, J.-M. Rost

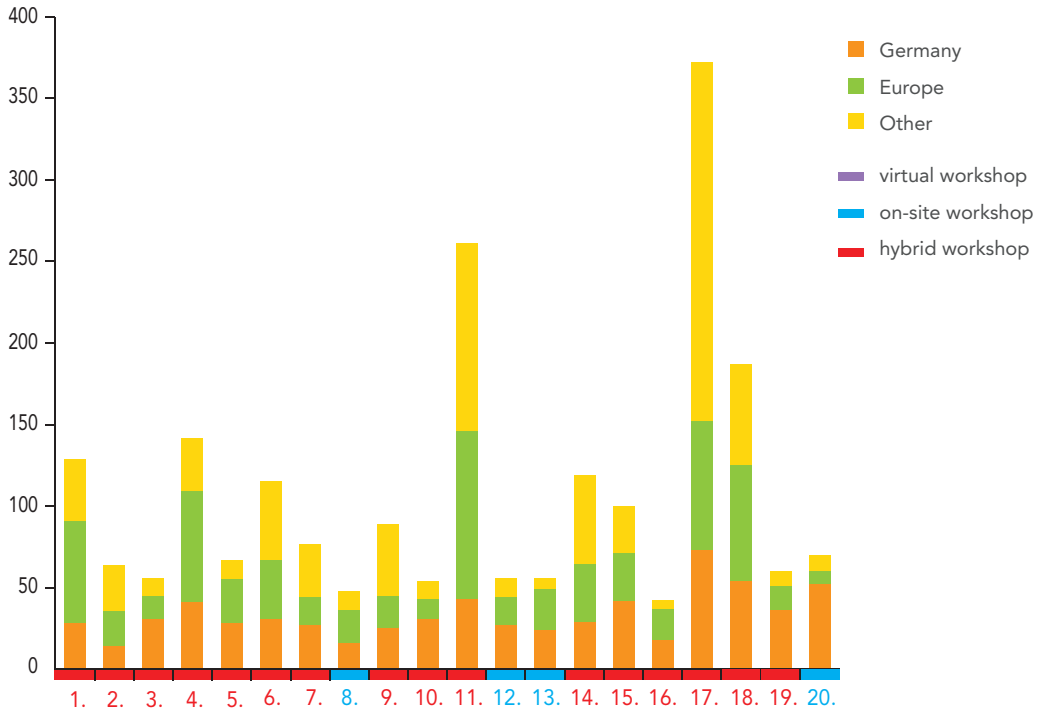
56. *Atomic Physics 2024*
Workshop: November 25 - 29, 2024 — 47 participants
Scientific coordinators: J.-M. Rost

57. *Localization and Constrained Dynamics in Quantum Many-Body Systems*
Focus Workshop: December 05 - 06, 2024 — 15 participants
Scientific coordinators: F. Heidrich-Meisner, R. Moessner, F. Pollmann

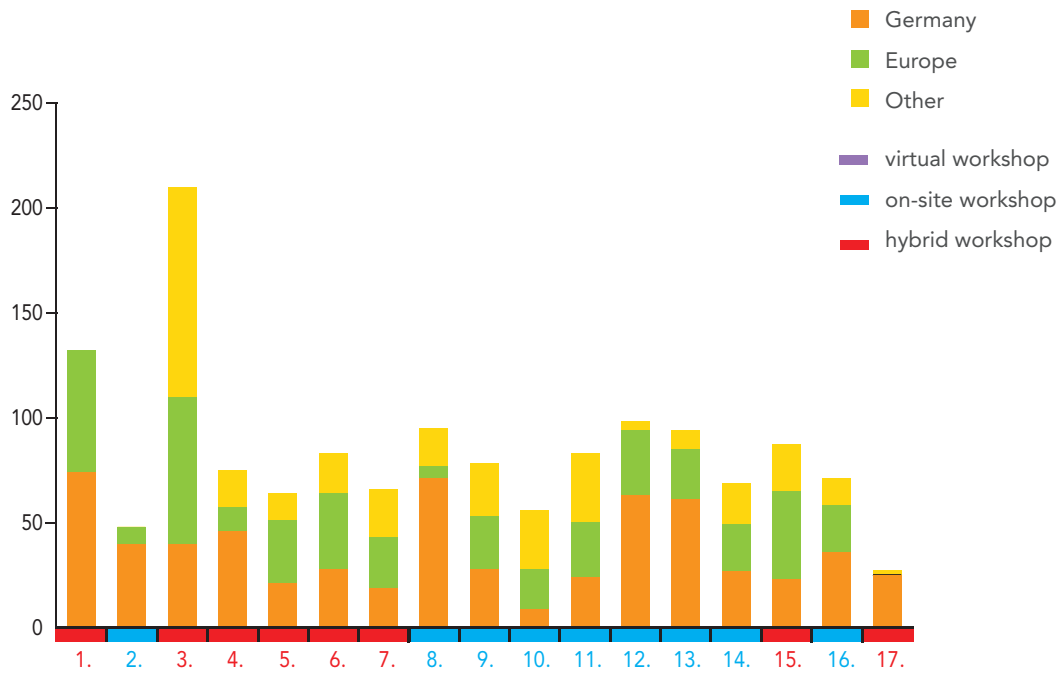
3.3.3 Workshop Participation



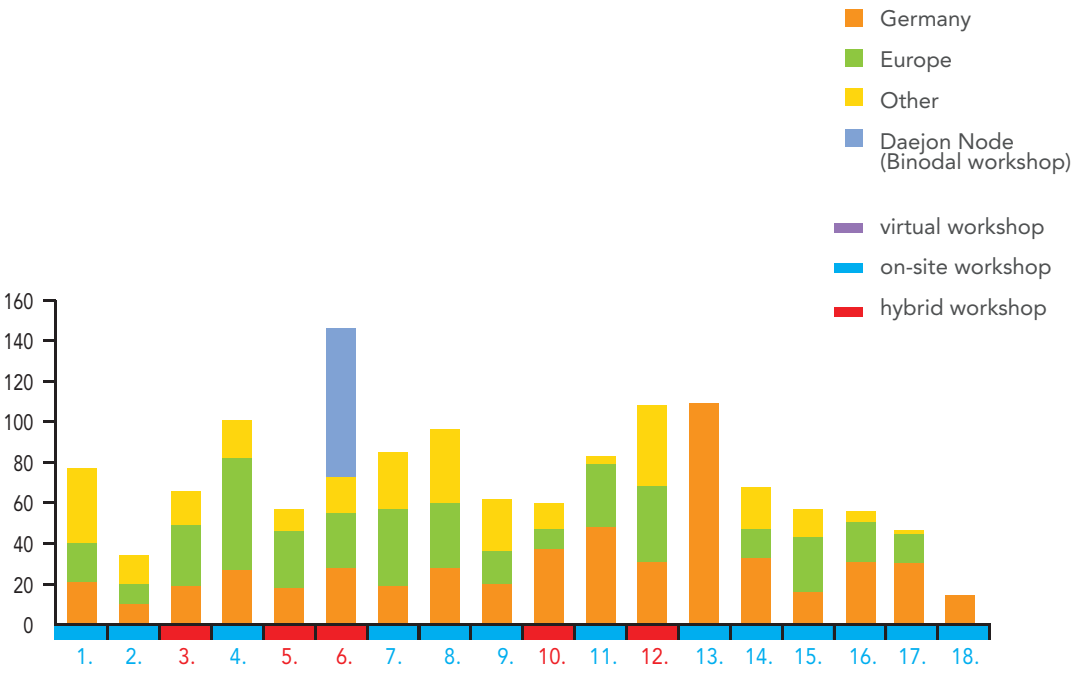
Number of Workshop/Seminar participants in 2021.



Number of Workshop/Seminar participants in 2022.



Number of Workshop/Seminar participants in 2023.



Number of Workshop/Seminar participants in 2024.

3.3.4 Workshop Reports

Ergodicity Breaking and Anomalous Transport in Quantum Many-Body Systems
Workshop
Scientific coordinators: A. Mirlin, F. Evers

The subject of the workshop was the quantum dynamics of many-body systems. The particular focus was put on the physics of many-body localization (MBL) and generalized hydrodynamics (GHD). These two rapidly developing fields have multiple connections: they address non-equilibrium physics of many-body systems that either completely break ergodicity or show very slow thermalization, and also exhibit anomalous transport. Further, experimental platforms and computational approaches to both classes of systems have much in common. Presentation at the workshop have also covered related research directions, including the physics of driven quantum systems as well of quantum measurements and the dynamics of quantum information.

The program included 35 invited talks, 11 contributed talks, and 33 posters. The total number of participants was 204, including 38 on-site and 166 virtual participants, representing 19 countries. On average, there were approximately 100 participants attending a scientific session, with peak values approaching 150. The program of the workshop included talks by a large number of leading experts in the field. At the same time, several invited talks, as well as the majority of contributed talks and of posters, were presented by young scientists who had an excellent opportunity to discuss their results with world-leading experts.

The workshop involved a balance participation of experimentalists and theorists. While a larger fraction of the talks were theoretical, there was a considerable number of experimental talks that covered essentially all key platforms -cold atoms, quantum spin chains, trapped ions, superconducting qubit arrays, disordered semiconductors- where the physics discussed at the workshop is currently explored.

In our view, the workshop was a highly successful event. It has offered a possibility for very fruitful discussions of the progress in the field and future perspectives. Each talk has been followed by a series of questions, answers, and comments. On many occasions, there were close connections between several talks that considered a related physics from somewhat different points of view, which has also prompted very instructive discussions. The meeting has stimulated various collaborations between the participants. We have received a feedback from many participants who pointed out that the workshop was very useful and stimulating.

The workshop was held in a hybrid format, which was an optimal solution in the present situation. In view of the COVID-related regulations, there was an upper limit 20 for the number of external on-site participants, implying a virtual format for the majority of participants. This was also inline with travel restrictions or complications for many participants, who would not be able to come to Dresden anyway. At the same time, it was extremely important to have a few tens of on-site participants, ranging from senior scientists to PhD students. This has permitted a very fruitful exchange of scientific ideas during numerous discussions between and after the scientific sessions.

We would like to thank the institute staff, and in particular Mandy Lochar, for outstanding organizational support. The possibility to organize the Workshop in the hybrid format has greatly contributed to its success. We are very thankful to Ronny Börner for invaluable support on the IT side.

Probing Complex Quantum Dynamics through Out-of-time-ordered Correlators
Workshop
Scientific coordinators: R. Jalabert, K. Richter

The workshop, initially planned for 12-16th October 2020, took place on 11-15th October 2021, with a hybrid format where one half of the speakers were present and the other half delivered their talk remotely. 34 participants (20+locals) were present on site and 136 scientists participated virtually, making it a highly international meeting with participants from 27 countries which encompassed the scientific leaders of the field, as well as many young scientists. A special place was reserved for PhD students and post-docs, with two central slots for poster sessions (in virtual format) and a further slot for a flash poster presentation (in hybrid format). The well-attended Monday colloquium was given by Prof. Roderich Moessner (mpi**pks**) on the subject of "Many-body chaos and order, through the lens of OTOCs" presenting the broad subject of the conference to the large community of Dresden physicists.

The workshop was markedly interdisciplinary, since the subject of OTOCs is of present interest to various fields and is linking usually scientifically disconnected research areas. We thus had participants from several Physics domains. Among them, quantum chaos, statistical physics, condensed matter physics, atomic physics, quantum open systems, and general relativity. Theory and experiment were both present in the talks and in the scientific discussions.

The recent advances in physics of OTOCs were discussed in the workshop, with a particular emphasis on issues related with many-body Quantum Chaos. While one-body Quantum Chaos is by now a mature discipline, with well-established results, its many-body counterpart is considerably less developed, given the difficulty to characterize the many-body quantum dynamics and the corresponding operator growth. The OTOC then appears as a highly valuable tool, since it allows for a characterization of the operator growth and information scrambling according to laws that are being explored. A particularly important development treated at the workshop comprised the universal bounds on the OTOC (referred to as "bounds on chaos"), and results concerning the conditions to reach these bounds were presented. The connection of OTOCs with the Eigenstate Thermalization Hypothesis, the Fluctuation-Dissipation theorem, and many-body localization were also established.

In addition, experimental realizations of OTOC protocols were discussed, as well as technical advances and challenges related with semiclassical approaches to OTOCs in the many-particle case. The important connection of the OTOC with holography and quantum gravity, which triggered the recent broad attention to OTOCs, was presented by several speakers, trying to bridge into the domain of Quantum Chaos. It is expected that such a connection will be further developed in the near future.

The success of the meeting would not have been what it was without the precious help of Mrs. Katrin Lantsch from the conference secretariat providing optimal administrative assistance during all stages of the organization, and of Mr. Ronny Börner providing perfect technical assistance for the remote participation. The organizers are particularly indebted to both of them.

Openness as a Resource: Accessing New Quantum States with Dissipation
Workshop
Scientific coordinators: S. Denisov, M. Campisi, P. Hänggi

The meeting was organized as a part of the advanced study group "Open Quantum Systems far from equilibrium" (2019-2022). The focus of the workshop has been chosen on the challenge to what extent the openness of a quantum system can impact the underlying dynamics in providing novel mechanisms and unforeseen phenomena for which a coupling of the considered quantum system to environments acts as a primary input; i.e., then evolving away from an unitary time-evolution, – in distinct contrast from its isolated dynamics. This being the case, openness presents not a nuisance but rather can be used as a resource: For example, non-unitary mechanisms such as dissipation and/or dephasing can be employed to fight decoherence in stabilizing new quantum states. Alike, those can be utilized to convert heat stemming from a coupling to environment(s) into useful work in quantum devices, allowing for the operation of thermal quantum machines, or also for the generation of stylized classes of new quantum states.

Despite the intricacies we faced with the still ongoing Covid-19 situation the meeting was planned from the very beginning as a hybrid format, but with all speakers taking part in the workshop strictly on-site, as well as all selected poster presenters. Consequently, the total number of on-site participants has been limited to no more than 30. This restriction together with the requirement of a full vaccination status in essence limited that the majority of those on-site participants were arriving from within Europe only. Altogether, a total of 130 participants took part at the meeting, including a total of 29 external on-site visitors plus a total of registered 101 virtual participants. All those could discuss, however, with the speaker(s) for both, those either attending on-site or in case for virtual participants via zoom during the respective on-site presentation and naturally also during the 10-15 minutes discussion round, which followed each presentation. The invited speakers included full professors, primary and senior post-docs, as well as selected PhD students actively engaged in the subject matter.

The agenda of the workshop was divided over a period of 4 days via selecting 4 main topics for each day: We started out with the the theme of periodically driven open systems – which culminated in an illuminating overview with the colloquium presented by Prof. A. Eckardt (TU Berlin). The next topic centered on nonequilibrium steady states of various open many-body systems. This was followed with presentations of many-body localization physics (in theory and experiment) and the challenging topic of

characterizing "Dissipative Quantum Chaos". The forth day was earmarked for quantum thermodynamics of general and specific open quantum systems, including a description for, – in parts still controversially discussed –, notions such as quantum work, heat and feedback-control in regimes from weak-to-strong system bath couplings. Somewhat off the main conference topic, a particular inspiring talk was presented by M. Haque who addressed the challenge of assigning a "temperature" to eigenstates of individual many-body states, via addressing all the pros and cons which this problem comprises.

In discussing with all participants we uniformly received praise for our chosen format: Particularly, our ample time provided for discussions between the oral presentations and during the poster session was highly appreciated. In several cases this initiated future ideas and in cases even instigated joint future collaborations among the participants. Particularly worth noticing was also the fact that the young invited speakers at their advanced PhD-level and primary postdoc-level presented most impressive talks that were rich in content and results.

Last but not least, the organizers like to thank the Institute staff, and in particular Mandy Lochar, for providing their dedicated and outstanding organizational support. The possibility to organize this very workshop in the hybrid format has greatly contributed to its success. We are very thankful to Ronny Börner for his invaluable support on the IT-side during the whole meeting. Likewise we thank the kitchen staff which provided very good tasting meals throughout all days of the meeting.

Ordinal Methods: Concepts, Applications, New Developments and Challenges
Workshop
Scientific coordinators: J. M. Amigó, K. Keller, O. Rosso

The workshop, initially planned for spring 2021, was held from 28th February to 4th March in a hybrid format with 64 registered participants from five continents, of which 15 were on-site participants from Brazil, Germany, Greece, the Netherlands and Spain, and 49 were virtual participants from 15 countries incl. New Zealand, Australia, China, Japan, Cameroon, Argentina, to name a few. A total of 42 talks were given, 15 by the on-site participants and 27 by on-line participants.

The key topics of the workshop concerned the application of the concept of ordinal pattern in different fields and theoretical aspects related to this concept. The topics discussed included permutation entropy, causality detection, ordinal networks, the entropy-complexity plane, and others. The workshop was highly interdisciplinary. It brought together researchers from different disciplines such as physics, mathematics, statistics, data analysis and computer sciences, interested in the theoretical aspects and practical applications of ordinal patterns, to discuss recent developments and challenges. The talks were supplemented by two discussion sessions, one on 'Ordinal Patterns and Machine Learning' and one on 'Statistical Aspects of Ordinal Pattern Distributions'.

With very few exceptions, the talks given in the workshop were of a high level, including those of newcomers who presented their work. A special highlight was the on-site colloquium lecture "Climate Meets Complex Systems: Exploring Predictability of Extreme Climate Events via a Complex Network Approach (on-site)" by Jürgen Kurths (Potsdam Institute for Climate Impact Research), presenting an overview of results of his working group. The on-site opening talk by Christoph Bandt (University of Greifswald) included interesting results and ideas for a further development of statistical methods based on ordinal pattern distributions. In some talks, the importance of ordinal networks to quantify complexity and coupling, as well as to detect causality was worked out. Moreover, impulses for new applications of ordinal patterns were given.

It is expected that this workshop will contribute to a further development of the field of ordinal patterns in the context of describing and investigating complex phenomena and data, particularly on the basis of newly established contacts and agreed collaborations. A Focus Issue of the journal Chaos on the topics of the workshop is being prepared to publish research papers and mini reviews, including work and ideas presented at the workshop.

Both from a scientific and social viewpoint, the workshop was very successful. This would not have been the case without the perfect organizational support provided by Dr. Michael Genkin and, particularly, Ms. Maria Voigt, and the perfect technical assistance by Mr. Ronny Börner regarding the virtual participation.

Physics and Collective Dynamics of Future Mobility
Focus Workshop
Scientific coordinators: M. Barthelemy, C. Sommer, M. Timme

The focus workshop PhyMo22 took place at the **mpipks** from March 9-11, 2022. We aimed at consolidating the interdisciplinary quantitative research on the collective dynamics and future challenges of sustainable human transport, both taking the perspective of Nonlinear Dynamics, Network Dynamics and Statistical Physics and respecting socio-economic and user boundary conditions. The workshop brought together more than 50 researchers working on different quantitative analyses and modeling aspects of human mobility with an emphasis on integrating theory and conceptualization, computational modeling and various approaches to data analysis.

New mobility services such as ride-sharing and ride-pooling constituted one major theme discussed. Theoretical and modeling analyses about optimal performance and suitable efficiencies of pooled or bi-modal services were contributed by Knut Heidemann, Charlotte Lotze and Steffen Mühle. David-Maximilian Storch discussed the potential of financial and other incentives for inducing a high fraction of ride-sharing adoption. Practical insights into the efficiency of on-demand ride-pooling systems were provided by Debsankha Manik of the Hamburg company MOIA, a dedicated branch of Volkswagen Group and the largest commercial ride-pooling service in Europe.

A second main topic was the overall characterization of traffic dynamics, with contributions, among others, by Thomas Guhr, Kay Axhausen and Marta C. Gonzalez. Several aspects of their conclusions were supported by large-scale data analysis. The planning of efficient transport networks such as bike paths and public transport networks was touched upon in the talks by Christoph Steinacker and Matthias Dahlmanns. Research towards the fundamental understanding of individual mobility behaviour was presented by Paolo Santi and Laura Alessandretti. Several other researchers, including Hugo Barbosa, David Levinson and Gourab Ghoshal, Michael Schreckenberg and Michael Szell, added their views in additional talks on topics like city transport infrastructure development or gender aspects of mobility. The workshop connected many established researchers with junior scientists. Participants actively engaged with each other's research and several repeatedly brainstormed, debated, or worked on open challenges after talks.

The scientific event concluded with a discussion about future physics research on mobility. Integrating micro- with macro-scale analysis was identified as one of the major research frontiers. Moreover, although machine learning often achieves excellent modeling results under given circumstances, it can hardly reveal causal mechanism underlying emergent phenomena, resulting in challenges in explaining policy decisions to transport users. Thus, complex systems research has been identified as becoming increasingly important for understanding intricacies, tipping points, phase transitions and new collective states, beyond what can be directly deduced from data.

Despite the ongoing COVID-restrictions and the event taking place in a hybrid format, the workshop succeeded in giving an impulse for collaborative research about understanding collective phenomena in transportation and contributing towards identifying a path towards sustainable mobility. We would like to thank the **mpipks** for offering the opportunity for the timely cross-disciplinary exchange, Katrin Lantsch for providing dedicated and outstanding organizational support and Ronny Börner for performing miracles on all IT tasks during the hybrid workshop. Thank You!

Topological Materials: From Weak to Strong Correlations
Focus Workshop
Scientific coordinators: S. Bühler-Paschen, T. Neupert, Q. Si

The Focus workshop TopCor22 took place from April 11-13, 2022 and brought together 145 participants (50 on-site + 95 virtual) from 19 countries. Its main aim was to foster exchange between two largely distinct communities working on the weak and strong correlation regimes of topological quantum materials, to highlight emerging unifying themes of topology across the correlation spectrum and stimulate new ideas.

The workshop featured a diverse line-up of speakers that covered a range of topics from experiment to theory, and from weak to strong correlations. For instance, Erik Sorensen and Hidenori Takagi gave illuminating updates on Kitaev spin systems, Yoichi Ando came with new data from Majorana heterostructures, Joseph Checkelsky focused on flat bands in kagome materials, Amalia Coldea introduced a method to extract information about Berry phases from quantum oscillation data, and Chandan Setty and Diego Zocco discussed the design and control of correlation-driven topological semimetals, while

Leslie Schoop and Claudia Felser added a chemist's view on materials discovery. Jennifer Cano proposed twist-tronics with topological surface states and Adrian Po reported on work in progress seeking to extend Jordan-Wigner transformations to higher dimensions. Annica Black-Schaffer gave the institute colloquium of the week, in which she pedagogically introduced concepts of topological superconductivity and discussed the emergence of phase crystals in boundary modes of high-temperature superconductors as an example of new correlation-induced phenomena. Two discussion sessions were integrated into the workshop. For these, participants were asked to hand in questions and comments in advance. The stimulating discussions, which engaged many participants, revolved around these questions, as well as selected topics that came up during the workshop talks.

The discussion sessions were also a great platform for junior participants to get involved and clearly demonstrated the advantages of the in-person format. Many PhD students used the opportunity for in-depth exchanges and networking. Alexander Tyner from Northwestern University summarized his experience as follows: „As a graduate student in my penultimate year, I found it to be a wonderful opportunity to both share my research and get a better sense of the directions others in the field have taken their research during the years of relative isolation [...]. In particular the discussion sessions and informal opportunities to discuss were greatly appreciated." Besides presentations at the poster session, a number of junior participants gave 5-minute contributed talks. They were of very high quality and nicely complemented the topics of the invited talks, by including, for instance, novel aspects of topological band theory or twisted van-der-Waals systems.

That the workshop indeed helped bridge the gap between the two communities is particularly highlighted in the two lively discussion sessions, with topics that came from both communities, such as

- To what extent does the shape/spread/topology of Wannier functions impact correlated instabilities?
- Strong correlations vs topology: when do they cooperate (in producing correlated topology), and when do they compete? Are there principles at play?
- Can parton type construction for correlated models be developed into ab initio methods for correlated topology?

The organizers came away from the workshop with the sense that continued dialogues between the communities and cross-fertilization of ideas will help explore and advance the unifying themes for electronic topology in disparate materials settings and across the spectrum of correlation strength.

The organizers thank the Institute staff, in particular Mandy Lochar for providing outstanding organizational support in these complicated times and Ronny Börner for his support with the brand new hybrid conference system, which helped to overcome the challenge of a 50 persons on-site cutoff!

Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers
Focus Workshop
Scientific coordinators: M. Hafezi, F. Pollmann, A. Smith

The mpi**pks** focus workshop Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers took place from 25-28 April 2022. It provided a platform for discussion of new approaches and advances in quantum computation and simulation with a focus on the use of near-term technology. The workshop was held in a hybrid-virtual format with around 60 participants, with the majority of talks given in-person. The format included 13 invited talks over the two and a half day program, with the addition of 12 short "lightning talks" contributed by the participants.

With the help of the hybrid format, the workshop hosted an international collection of speakers from the USA, Australia, Israel, UK, and across Europe. The senior speakers and participants are among the leading scientists performing cutting-edge research in the scope of the workshop. Importantly, the majority of the high quality contributed lightning talks were from young researchers.

The junior participants were a core component of the workshop. Not only those giving excellent presentations, but also by actively engaging in discussions in breaks and during the workshop dinners. It was a great pleasure to meet researchers, both new and established, in this growing field.

Given the high quality contributions from both senior and young researchers from around the world, and the accompanying active discussions, we believe the goal of the workshop was clearly achieved. The breadth of the topics within this focus area - covering theoretical and experimental aspects of digital and

analogue quantum computation, simulation, and quantum information - demonstrates how the workshop successfully brought together the wider research community in this field.

Emergent Hydrodynamics in Condensed Matter and High-Energy Physics
Workshop
Scientific coordinators: A. Gromov, D. Son, P. Surowka

The focus of this workshop was on the hydrodynamic behavior and its microscopic origin of topological, fractonic and active matter. Phases of matter consist of collective states of particles that have emergent properties beyond their underlying microscopic constituents. They can be divided by the nature of their excitations with vanishing energy. We distinguish gapped systems that do not have excitations as the energy goes to zero and gapless systems with zero energy excitations in isolated points in momentum space. Examples of gapped systems include insulators and quantum Hall states. Gapless systems comprise of semimetals such as graphene and Dirac/Weyl semimetals or certain newly discovered fractonic phases of matter with immobile excitations. Their exotic properties are believed to be at the heart of new generation of electronics (semimetals), novel type of quantum memories (fractons) or future engineering (metamaterials). Ultimately the research goals were to understand the interplay between symmetry, topology and geometry at different scales and connect transport phenomena to microscopic models.

We gathered prominent experimentalists and theoreticians from around the world. The top experimental groups in the field of electronic hydrodynamics were represented by Andrew Mackenzie, Shalal Ilani, Yuan Yan, Jonah Waissman. The main theoretical physicists present included Alexander Abanov, Anton Burkov, Joel Moore, Jörg Schmalian, Igor Shovkovy, Michael Stone and Vincenzo Vitelli.

We had several young researchers present, who reported their results as speakers (Paweł Matus, Jimena Siepe) and in the form of posters. All of them showed scientific maturity and good outreach skills.

The workshop served as a platform to connect communities of condensed matter and high-energy physicists. Both communities are actively investigating hydrodynamic regime of matter. In the high-energy the focus is on heavy-ion collisions and in condensed matter on topological materials and metamaterials. The workshop provided an opportunity to report new technical developments in kinetic theory, hydrodynamics and effective field theories as well as discuss a variety of physical systems and phenomena, in which new transport signatures can be present. As a result, researchers will be able to, on the one hand, extend the applicability of the developed formalisms and on the other hand to identify proper theoretical description to the experimentally observed phenomena.

Chimera States: From Theory and Experiments to Technology and Living Systems
Workshop
Scientific coordinators: J. Davidsen, Y. Maistrenko, K. Showalter

One of the pillars of modern physics is the concept of symmetries. Spontaneously breaking such symmetries typically gives rise to non-trivial phenomena and can explain, for example, why particles have mass. The occurrence of such symmetry-breaking phenomena is not limited to particle physics but occurs across a wide range of physical, chemical and biological systems. Recently discovered examples include chimera states. Chimera states are hybrid states characterized by the coexistence of localized synchronized and unsynchronized dynamics in a given system. Indeed, the name chimera is used here in direct analogy to the hybrid creature in Greek mythology. Such coexisting behavior can even occur in a homogeneous system, thus breaking the underlying symmetry — something that was long thought to be impossible. While over the last 20 years a significant theoretical understanding of this phenomenon has started to emerge, experimental realizations remain scarce and the relevance of the phenomenon in technology and in nature remains to be established – leaving many challenges and fundamental issues to be addressed.

Chimer22 targeted many of these questions. These included but were not restricted to:

- Do chimera states control biological and/or cognitive functions?
- Do chimera states play any significant role in natural biochemical mechanisms?
- In which natural or experimental systems does an effective nonlocal coupling naturally arise?
- Do chimera states exist all the way down to the quantum scale?
- What technological advantages do chimera states offer?
- Which experimental systems are most promising to study chimera states in three dimensions?
- How can we establish the existence of chimera states in continuum systems experimentally?

Chimer22 invited 23 outstanding experts in this area of research from all over the world, of whom 16 participated in person. To name only a few of the key attendees, who contributed to the big success of Chimer22 by triggering and facilitating discussions and new collaborations, we list:

- Rajarshi Roy: Coherence, Chimeras and Passage Time Statistics in Light,
- Katharina Krischer: Chimera states, coexistence patterns and multifrequency clusters in systems of nonlinearly coupled amplitude oscillators,
- Ying-Cheng Lai: Chaos in Dirac electron optics: Emergence of a relativistic quantum chimera,
- Christoph Bruder: Quantum synchronization,
- Kanika Bansal: Chimera states in human brain network models,
- István Z. Kiss: Weak Chimera States in Modular Electrochemical Oscillator Networks,
- Eckehard Schöll: Controlling chimera states in complex networks: interplay of dynamics, network topology, and time delay,
- Erik A. Martens: On the Origin of Chimera States in Mechanical Systems.

In particular, young investigators and researcher from related disciplines were given the chance to present their work, which included a successful poster session. Several discussions and new collaborations were facilitated through this. Overall, Chimer22 had 74 registered participants with 44 on-site participants incl. 2 organizers from Germany, Canada, Hungary, Poland, Singapore, the US, Ukraine, Switzerland, Sweden, Japan and India and 30 virtual participants from 16 countries incl. New Zealand, Australia, Cameroon, Korea, Canada, India to name a few. Out of the 42 talks, 10 were presented virtually and 32 in person.

The key scientific result of Chimer22 is most certainly the various novel collaborations that emerged from the in-depth in-person discussions. These collaborations will result in various publications and research grants. Already during the workshop, researchers who had not worked together joint forces to tackle some of the challenges mentioned above. A forthcoming Focus Issue in the journal Chaos will cover the topics of Chimer22 and include papers by leading scientists participating in the workshop.

Quantum Chaos and Holography
Workshop
Scientific coordinators: H. Liu, A. Polkovnikov, M. Rozali

The main purpose of this workshop was to facilitate an intensive exchange of ideas between string theorists, condensed matter physicists, atomic physicists, mathematical physicists and researchers with other areas of expertise actively working on theory and applications of quantum chaos. It served a dual goal of both introducing researchers from different communities to key models and results and outlining unresolved problems actively investigated by these different communities.

Key speakers:

- Prof. Alexander Altland (Universität zu Köln)
- Prof. Micha Berkooz (Weizmann Institute of Science)
- Prof. Johanna Erdmenger (Julius-Maximilians-Universität Würzburg)
- Prof. Ben Freivogel (University of Amsterdam)
- Prof. Olivier Giraud (LPTMS Orsay)
- Prof. Stefan Kehrein (Georg-August-Universität Göttingen)
- Prof. Tomaz Prosen (University of Ljubljana)
- Prof. Marcos Rigol (The Pennsylvania State University)
- Prof. Julian Sonner (University of Geneva)

The conference featured a large fraction of young participants postdocs, graduate students and junior faculty. We accepted oral presentations from all postdocs and junior faculty, who requested to give a talk. One graduate student substituted Prof. Adolfo Del Campo, who could not come for personal reasons, and also gave an oral talk. All other graduate students were given an opportunity to present a poster. All junior participants, as far as we can judge, actively participated in multiple discussions during the conference. The organizers allocated extended time for such interactions.

The conference connected very different communities and facilitated exchange of a very broad range of ideas between them.

Band Topology in Quantum Magnets: From Nontrivial Excitations to Non-Hermitian Topology and Spintronics
Focus Workshop
Scientific coordinators: P. A. McClarty, J. G. Rau, J. Romhányi

The focus workshop TOPMAX22 which took place June 13-15, 2022 brought together 88 participants (34 on-site, 54 virtual) from 17 countries working on topological excitations in magnetic systems. Our goal was to address the key challenges and questions in this rapidly developing field and to develop connections to the adjacent fields of quantum magnetism, spintronics, non-Hermitian topology, the dynamics of complex spin textures, and electronic topological materials coupled to magnetism.

The workshop included talks from many of the key contributors to this new and growing field. We highlight:

- Alexander Chernyshev: who kicked off the meeting with pressing questions on the effect of strong magnon interactions on topology
- Marcus Garst: who presented the first evidence for emergent Landau levels in the magnon excitations of a skyrmion crystal.
- Yuan-Ming Lu: who provided a framework for discovering topological magnon materials based on Topological Quantum Chemistry
- Alexander Mook: who discussed the role of magnon bound states in enhancing the possible topological magnon states

We structured the workshop to create opportunities for junior scientists to present their recent work as contributed presentations. These were generally excellent talks, addressing timely questions, and initiating productive discussions. In particular, we call attention to: Miska Elliot who spoke about recent work on the observation of Dirac magnons in a stacked honeycomb system and Peter Czajka who provided tantalizing evidence for topological magnons underlying the perplexing thermal Hall signal observed in α-RuCl3.

The workshop opened a range of lively discussions on several key questions in the field of topological magnetic excitations:

- Does magnon band topology survive the presence of interactions? (such as quasi-particle decay).
- How can we experimentally detect topologically protected magnon surface states in real materials?
- Can topological magnons play a role in generating or controlling spin currents that may be useful for spintronics?

The meeting provided the first face-to-face forum for discussing issues in this developing field and provided considerable food for thought. The organizers look forward to a further iteration of this meeting in the hopefully near future once some of the current challenges have been met.

The organizers would like to express their appreciation to the staff at mpi**pks**, including the cafeteria and guest house staff. We also thank Ronny Börner for his technical assistance with the hybrid conference system that enabled the seamless participation of our online attendees and contributors. We would like to especially thank Mandy Lochar for her remarkable organizing skills and patience, without which this meeting would not have been possible.

Intelligent Machines? – Self-Organized Nonlinear Dynamics of Machines across Scales
Workshop
Scientific coordinators: N. Hoffmann, P. Manoonpong, M. Timme

The international workshop InteMa22 took place at the mpi**pks** from June 20-24, 2022. The aim of the event was to bring together researchers from nonlinear dynamics and complex systems science with those from smart systems' and robotic engineering and artificial intelligence to further our understanding of the dynamics of complex multi-dimensional machines – specifically those that themselves shall exhibit forms of smartness or intelligence. The workshop had 30 participants working in the areas of mechanical systems, smart materials, neural networks and learning systems as well as complex information processing and communication systems and concepts.

Investigating the ability to efficiently move and interact with complex environments was one of the major themes discussed at the workshop. Auke Jan Ijspeert presented a series of models demonstrating how robustness to neural disruptions can be achieved in robotic locomotion. Using machine learning for adaptive interlimb coordination in bio-inspired robots was the topic of Poramate Manoonpong's talk, while Bulcsu Sandor offered insights into creating a network of neural oscillators for generating hexapod-type motion patterns. Maziar Ahmad Sharbafi and Philipp Rothemund explained solutions aiming at improving robot/smart device interactions with the environment. Contributions to the topic were made also by Je Min Hwangbo, Thies H. Büscher, Claudius Gros and Xiaofeng Xiong. Short-term, few-shot learning and the mechanisms underlying the learning dynamics has been identified as one of the overarching open topical questions.

A second most relevant topic was (self-)organization in multi-agent systems. At the workshop's colloquium, Metin Sitti presented a self-organizing robotic collective system at the microscale capable of having interactions inducing various nonlinear coupled dynamics and dynamic self-assembly modes. Christian Bettstetter discussed in his talk a proof of concept for a multi-robot system of small ground robots and drones that forms emergent space-time patterns. Self-organized distributed patterns in the collective response dynamics of fluctuation-driven power grids was the topic of Xiaozhu Zhang's talk. The many different aspects of the workshop's topic were reflected in the talks' diversity: smart materials (Thomas Wallmersperger, Zhenwu Wang), smart particles (Holger Stark), new approaches to computing (Lucas Wetzel, Wei Lu, Yulia Sandamirskaya), apps for sustainability awareness (Johannes Klinglmayr), etc.

The workshop connected many established researchers with junior scientists. Participants actively engaged with each other's research and several repeatedly brainstormed, debated, or worked on open challenges after talks.

Despite the event taking place in a hybrid format, the workshop succeeded in giving an impulse for collaborative research. We would like to thank the mpi**pks** for providing the opportunity for this highly relevant cross-disciplinary exchange, Maria Voigt for providing dedicated and outstanding organizational support and Ronny Börner for performing miracles on all IT tasks during the workshop. Thank You!

Dynamics of Immune Repertoires: Exploration and Translation
Seminar and Workshop
Scientific coordinators: A. Eugster, U. Hershberg, M. Or-Guil, G. Yaari

Main focus and key participants. The Dynamics of Immune Repertoires international workshop and seminar was comprised of six interlinked working groups and one 5-day seminar. Due to the pandemic, we were gifted a very long planning period. This allowed us to integrate between relatively disparate topics that together underlie the knowledge we are missing in the study of immune repertoire dynamics. We also took advantage of the enthusiasm of our different research communities to return to interact face to face following the disconnection of the pandemic. Thus, we were fortunate to find 12 brilliant leaders in their field to organize the six working groups studying: - (in chronological order but in equal importance) – WG1: "T cell trajectories and TCR diversity in health and disease", WG2: "Evolutionary footprints in immunoglobulin V genes", WG3: "The primary B-cell immune response", WG4: "Machine learning in computational immunology", WG5: "Evolutionary scales of the immune system", and WG6: "Can TCR specificities be predicted?". We were also able to cover these topics with many talks by senior, established researchers in those fields during the seminar week, offering participants a very broad overview over this still very dynamic field.

Integration of newcomers and new ideas. The co-operation of our workshop organizers allowed us to invite both the key players as well as newer emerging researchers in each field, to both, the workshops and the seminar week. Our ability to allow (some of the) participants to stay throughout multiple working groups as well as the week-long seminar enabled a cross topic integration of ideas. All 4 scientific advisors come from multidisciplinary backgrounds and so we were very aware of the need for education to discussions across disciplines. Thus, we encouraged participant to exit their comfort zones and attend both the more computational WGs (4 and 6) and the more experimental biology WGs (1,2 3 and 5). In addition, we ensured the poster session included early studies incorporating both computational and experimental aspects of immune research.

Wider scientific impact. IMMREP22 had several general and concrete impacts. First and foremost, it extracted our scientific community from the doldrums induced by the isolation of COVID-19. It also opened several novel avenues of research stemming from each of our WGs. WG1 described a new comprehensive theory for T cell dynamics in health and disease; WG2 started an initiative to create a novel

method for V(D)J segment verification and annotation allowing for easier, less centralized and more coherent integration of community findings; WG3 resulted in a more integrated multi scale view of initial immune responses from which a review of key facts and open questions is being created. WG4 has re-invigorated the field of artificial immune systems leading to a new series of workshops starting in the summer of 2023, as well as a special issue in Immunoinformatics. WG5 re-integrated ideas from comparative immunology into our main-stream human and murine focused understanding of immunity. WG6 made several important advances in our understanding and ability to model T cell specificity and kicked off an ongoing collaboration. (Initial results published here: https://doi.org/10.1016/j.immuno.2023.100024). Together, all working groups have shown the power of a multidisciplinary approach focused on the study of diversity and dynamics in immunology and biology in general, and resulted in scientific papers and new and exciting initiatives and collaborations.

New Trends in Nonequilibrium Many-Body Systems: Methods and Concepts
Workshop
Scientific coordinators: F. Heidrich-Meisner, T. Oka, P. Werner

Scope and Focus. NEQMBS22 aimed at bringing together experts working on nonequilibrium physics in quantum-many body systems and materials, with a focus on newly developed theoretical methods and concepts. The workshop covered Quantum Monte Carlo techniques, Green's function methods, matrix-product state methods, techniques for electron-phonon coupled systems, and Floquet systems. The theoretical talks were complemented by five experimental talks on recent progress in nonequilibrium studies of 2D materials, magnetic systems, 3D Dirac materials, and quantum simulators.

Participants. Due to Covid related restrictions, the participation was limited to at maximum 60 participants. We admitted 56 participants (incl. 3 organizers) from Austria, Colombia, Germany, India, Japan, Switzerland, the US etc., just to name a few. The workshop program featured 41 talks, including a colloquium, and 11 poster presentations. The colloquium given by Monika Aidelsburger, LMU, attracted an additional virtual attendance of 25 persons. Outstanding participants in the workshop were, on the one hand, the senior experimentalists U. Bovensiepen and R. Shimano as well as our colloquium speaker, M. Aidelsburger, and on the other hand, key theory speakers including M. Eckstein (electon-phonon problems in DMFT), A. Polkovnikov (closed quantum systems), E. Gull (improved techniques for spectral functions), F. Pollmann (constrained dynamics), M. Sentef (light-induced superconductivity), T. Morimoto (nonlinear optical effects) and G. Stefanucci (nonequilibrium Green's functions). The more junior experimentalists (D. Bossini and M. Reutzel) gave excellent and well-received talks on ultrafast amplification and nonlinear coupling of coherent magnon nodes and excitons in Moire systems, respectively. The workshop featured a large number of 22 contributed talks with many early-career scientists presenting. The work on a matrix-product states representation of the influence functional and potential applications to quantum impurity problems by Lerose triggered significant discussions. D. Golez spoke about promising new ideas to compress nonequilibrium Green's functions. The poster session was well attended and triggered very active discussions. Overall, the decision to hold the workshop in a purely onsite format and to leave enough time for coffee breaks and informal discussions resulted in very active and sustained exchanges among the participants. mpi**pks**'s excellent support infrastructure made the participation of two scientists with small children possible and the overall organization was perfect, as always, which is highly appreciated.

Scientific results. The workshop highlighted both impressive progress as well as significant challenges in the theoretical description of quantum many-body systems in the nonequilibrium regime. Pushing accessible time scales forward at manageable computational cost is a main theme and progress was reported for nonequilibrium Green's functions, DMFT methods, and MPS techniques. Moreover, improved techniques to obtain spectral functions from real-time data as discussed in the workshop may facilitate the link to experiments. We expect that the lively discussions during the workshop have stimulated new ideas and collaborations, so that this meeting at mpi**pks** will contribute to the future progress in the field of nonequilibrium many-body systems.

Shedding Quantum Light on Strongly Correlated Materials
Workshop
A. Imamoglu, D. Jaksch, F. Piazza

Title of the event. "Shedding Quantum Light on Strongly Correlated Materials"

Main focus of the workshop. This workshop aimed at identifying new research directions, as well as developing a comprehensive framework for constructing, probing, and modelling strong-coupling QED in correlated quantum materials, thereby establishing a common ground for physicists working in the fields of quantum optics and condensed matter.

Most important participants. The participants who should have mostly profited from this workshop are the students and young postdocs, through being exposed to the cutting edge research in this field from both the perspective of solid-state and atomic gases perspective. We hope this will help them building a specific profile at the border between communities.

How did scientific newcomers present themselves. Roughly one third of the talks were contributed by young applicants. We allotted the same amount of time for contributed talks as for invited talks. We were impressed by the clarity of presentation and quality of the results of all the contributed talks.

Scientific results of the workshop in the broader sense. It was important for us to have in-person workshops after the pandemic break, especially given the young and quickly developing field. For this reason, we decided to have the workshop fully on site, with plenty of time for discussions. One main result has thus been to provide an avenue for direct and extended scientific and personal interactions.

A second main result has been that these interactions took place across communities, between scientists that had never met before, and in several cases did not know about relevant research overlap.

We hope that this workshop will be a positve example and trigger future similar events merging the communities of quantum optics/atomic physics and solid-state physics under the common denominator of QED within materials.

Quantum Transport with Ultracold Atoms
Workshop
Scientific coordinators: H. Ott and S. Wimberger

The workshop was a great success, also thanks to the extremely efficient organisation and support by the visiting program of the mpi**pks**, in particular we mention Mandy Lochar, Michael Genkin and Ronny Börner. It hosted 56 onsite participants from all continents, speakers from 17 countries, and over 60 virtual participants. Our onsite participants included 10 women with 9 active contributions in form of talks or posters. Even the strike of a main air carrier on Friday was handled very flexibly by reshaping only slightly the program on Thursday afternoon that allowed some participants to leave early. We thank all participants for their collaboration and the high presence even on the last day with more than 30 persons onsite. From all the feedback that has reached us so far, our workshop seems to have been very attractive from the scientific point of view but also for connecting people. We thank all the participants for their active contributions, also during the extended discussion periods. Most of the participants enjoyed being together in a real-life meeting for the first time after the pandemic outbreak in 2020.

We highlight a selection of considerations that contributed to the success of the Workshop:

- Only four out of 36 talks were given virtually, in each case due to personal reasons impeding travelling. Our insistence on onsite participation turned out to be vital for guaranteeing such a high number of people actually present.
- Talks were divided into a three different formats, nine keynote talks of 50+10 minutes dedicated to the presentation of different experimental platforms, 15 invited talks of 35+10 minutes (theory and experiment mixed), and 12 contributed talks of 20+5 minutes. Additionally, we had two evening sessions for the 23 poster contributions. This led to an intense but diverse program with many occasions for discussions in the lecture hall and during the breaks. From the keynote talks we just mention representatively the mpi**pks** colloquium by Giacomo Roati (Florence), and the talks by David Guery-Odelin (Toulouse), H.C. Nägerl (Innsbruck), and David Weld (Stanford) that brought to us the highlights from the labs worldwide. Young researchers at the postdoc level were included in all categories, while (PhD) students were mainly represented during the poster sessions. Due to the rather generous time slots for the talks, there was always enough time for discussions without delaying the workshop schedule.

- Much positive feedback has been received on the equal mixture of experimental and theoretical contributions, both during the talks and the poster sessions. This was originally planned as such and proved crucial to the conference's success.
- The hiking tour on Wednesday afternoon gave to ca. 45 participants the chance to discuss informally about physics and beyond. We found that this event created many new links between the participants showing up in lively discussions the next two days. We are sure that our Workshop has created not just more understanding between the various aspects of quantum transport with cold atoms but also a momentum for future collaborations between the participants. This success and the perfect organisation by mpi**pks** make as plan a follow-up event, possibly on the topic of localisation and delocalisation in quantum systems, as a natural new focus after our transport conference. Consequently, the Workshop has created new impetus towards new developments in the field of nonequilibrium transport with ultracold atoms and beyond.

Inverse Network Dynamics - Network Structure and Function from Nonlinear Dynamics and Time Series Data

Seminar and Workshop

Scientific coordinators: K. Lehnertz, M. Nitzan, M. Timme

NetDat22 took place at the mpi**pks** from September 12-21, 2022. The aim of the event was to bring together theory and method development on inverse problems in network dynamics, on the rapidly evolving topics of network structural inference and on the network design for desired dynamics, as well as their numerous fields of application. The workshop had almost 100 participants from 19 countries working in the areas of nonlinear network dynamics, time series analysis, statistical inference as well as machine learning and data-driven modeling. Given the event has been rescheduled and newly planned twice from 2020 to 2021 to 2022, we adapted the original schedule of starting with 2.5 days seminar lectures followed by a week of workshop about new research results. To accommodate time constraints by the speakers (in part online, in part on-site), the event offered seminar sections distributed across the entire 1.5 weeks. Here, several established researchers presented introductory material about the full range of topics: higher-order interactions in multi-dimensional dynamical systems, universal aspects of network dynamics, inference of oscillator responses from probing experiments, approaches and challenges for the inference of various functional, effective or structural network from data, and a guided tour to (deep) machine learning for non-machine learning researchers, among others.

Many eminent contributors, along with young scientists, presented their topical research findings in the workshop parts. Common topics included the dynamics of (and near) tipping points and their prediction, avoidance as well as recovery of normal or desired operating states; the conservation of Granger causality by suitable compressed sensing matrices, interpretable machine learning for learning network structure; the inference of network size and structure based on multiple transient time series; the mathematical option space for reconstructing network topologies from the time series of their node dynamics by sparse regression; and the quantification by a sensitivity measure for inference problems by bridging exact mathematical work with physics-style exploration for cases not tractable analytically. Posters were available also after a poster session catalyzing several additional discussions.

NetDat22 had a big contribution towards community building, as indicated by many lively discussions not only at the dedicated discussion sessions, but also during the coffee breaks, lunch or dinner as well as a discussion dinner self-organized by the participants on the final evening of the event. The event took place in a hybrid format, yet the workshop succeeded in giving a strong impulse for collaborative research. The participants appreciated the topical breadth of the program. Many excellent presentations of the different approaches developed across wide-spread application fields generated an extraordinary number of interactions between participants from different fields and backgrounds, initializing new international and interdisciplinary collaborations.

We would like to thank the mpi**pks** for providing the opportunity for this highly relevant cross-disciplinary exchange, Katrin Lantsch for providing outstanding organizational support and Ronny Börner for using NetDat22 insights and more on all IT tasks during the workshop. Thank You!

QED Laser Plasmas
Workshop
Scientific coordinators: A. Di Piazza, S. Mangles, M. Marklund

The workshop QED Laser Plasmas (QLASP22) was originally planned to be held in September 2020 but then postponed until September 2022, due to the outbreak of the COVID-19 pandemic. The aim of the workshop was to bring together the two laser-plasma and strong-field QED communities, to explore the rapidly growing new field of nonlinear relativistic multi-particle quantum dynamics. The workshop was initially conceived mainly by Dr. Felix Mackenroth, who then left the research after the workshop proposal was accepted. We remaining three coordinators decided to keep the list of invited speakers as well as the concept of the workshop as much unchanged as possible as those agreed together with Dr. Mackenroth.

Forty two persons participated in the workshop (including the three coordinators) from mostly Europe (Germany, Poland, Portugal, France, Romania etc.) but also from South Korea and the US. The workshop included 37 talks, 20 of which were invited. Also, 32 talks were held in person and 5 held virtually, with one cancellation.

The workshop was characterized by clear and exciting talks as well as by very lively Q&A sessions, with discussion often continuing during the coffee breaks and the lunch/dinner breaks. Several interesting topics were discussed like the influence of nonlinear relativistic quantum dynamics onto ultra-intense laser-plasma interactions, how multi-particle plasma effects affect nonlinear relativistic quantum dynamics, and which experimental tests can explore relativistic quantum plasmas.

A distinctive feature of the workshop, as compared to previous similar events, was the relatively numerous experimental talks on planned and/on already performed experiments in strong-field QED. In this respect, world-leading experts representing high-power laser facilities (Prof. Matt Zepf for the CALA facility in Germany, Prof. Liangliang Ji for the SEL facility in China, Dr. Mohammad Mirzaie for the CoReLS facility in South Korea, and Dr. Petru Ghenuche for the ELI-Beamlines facility in Romania) presented exciting prospects and sometimes also preliminary results on experiments involving laser intensities beyond 10^{20} W/cm^2. This has clearly shown that soon dedicated experimental campaigns in strong-field QED will be realized world-wide (the recent exciting progresses made by the E320 collaboration and the corresponding experiment at SLAC in California (US) was reported by Dr. Elias Gerstmayr).

From the theory side, world-recognized experts like Prof. Alexey Arefiev, Prof. Sergei Bulanov, Prof. Christoph Keitel, and Prof. Tito Mendonca, together with younger and already renowned scientists like Dr. Stepan Bulanov, Dr. Nina Elkina, Dr. Arkadi Gonoskov, Dr. Mickael Grech, Dr. Felix Karbstein, Prof. Katarzyna Krajewska, Dr. Daniel Seipt, Dr. Matteo Tamburini, and Dr. Marija Vranic presented new developments on a broad class of phenomena including spin effects, collective effects, pathways to reach higher-and-higher intensities towards the Schwinger limit, strategies to observe electron-positron pair production, as well as sophisticated numerical techniques and methods to model upcoming experiments in strong-field QED.

During the Q&A sessions it has clearly emerged that different groups will probably start scientific collaborations and links between experimental and theory groups were initiated. Thus, we are convinced that the workshop was a successful event and represented the first meeting in our field, where it clearly emerged that experiments in strong-field QED will be pursued world-wide by several groups. Another important result, in our opinion, was the evidence that theoretical groups are making both continuous efforts to improve analytical and numerical methods to prepare the analysis of upcoming experimental results and exploring new regimes and effects to be ultimately also verified experimentally. All in all, the lively atmosphere of workshop and the extensive constructive discussions reflected the present excitement of the strong-field experimental and theoretical communities, and significantly contributed to build bridges between them, which will certainly push forward the development of our field.

Topology and Non-Equilibrium Dynamics in Engineered Quantum Systems
Workshop
Scientific coordinators: M. Aidelsburger, A. Eckardt, W. Hofstetter

The workshop "Topology and non-equilibrium dynamics in engineered quantum systems", organized by and at the Max-Planck-Institute for the Physics of Complex Systems (**mpipks**) in Dresden together with the DFG Research Unit FOR2414 on "Artificial Gauge Fields and Interacting Topological Phases in Ultracold Atoms", was a great success. Thanks to the highly professional organization and great commitment by

Mandy Lochar and the excellent technical support by Ronny Börner, more than 184 participants (61 on site as well as another 123 online) enjoyed inspiring presentations covering diverse subjects at the boundary between non-equilibrium quantum dynamics on the one hand and topological aspects of quantum systems on the other. In total 16 invited and 13 contributed talks reported both on theoretical and experimental results. Thanks to the rather large number of contributed talks (30 minutes including discussions), the workshop could raise the visibility especially also of young participants. To further enhance interactions between participants there were two poster sessions on Tuesday and Thursday evening, as well as an excursion to Meißen and a conference dinner on Wednesday. Topics that were covered in this workshop include, inter alia, the Floquet engineering of topological states of matter, non-Hermitian quantum systems, topologically-ordered states of matter, the robustness of topological properties under quantum quenches and the topological properties of open quantum systems. Moreover, diverse experimental platforms of engineered quantum systems, were addressed, such as ultracold atomic quantum gases, superconducting qubits, moiré materials and exciton-polariton systems. Lively discussions both after the presentations, during the poster sessions and during the breaks were observed and, hopefully, inspired fruitful future research.

Interdisciplinary Life of Microbes: From Single Cells to Multicellular Aggregates
Workshop
Scientific coordinators: L. Chai, E. Shank, V. Zaburdaev

This meeting was devoted to the topic of bacterial biofilms, which, from a biological perspective, can be naively described as "just" a community of bacteria encapsulated in a polymeric matrix that form on surfaces. The complexity and heterogeneity of cell phenotypes and their interactions make biofilms versatile and robust in response to environmental stresses and render biofilms untreatable in cases where they colonize medical devices, where they can be almost unremovable. Understanding this phenotypic and structural complexity is only possible by a coordinated interdisciplinary approach, facilitation of which was the goal of our meeting.

Central to achieving this goal was to attract the world-leading experts in biofilm research, but also from neighboring disciplines, as broad as medicine, chemistry, theoretical and experimental biophysics, and microbiology. More than 70 % from the first preliminary list of speakers did come to Dresden to report on their latest results and participate in extensive discussions. The colloquium given by Roberto Kolter (Harvard Medical School) provided an impulse of novel ideas that echoed across many key presentations during the workshop: hypothesis for biofilms as a part of human oral tissue (M. Hannig), role of antimicrobial peptides in disease (C. Bogdan, G. Wong), mechanical forces and their sensing (V. Gordon, N. Biais), regulation of bacterial metabolism (R. Hengge) and bacteria/yeast interactions in caries (K. Drescher), just to name a few. Seven presentation slots were allocated to contributed talks, which were supplemented by the two well-attended poster sessions. On the first day the poster jury selected the best posters and on the second day, the poster presenters themselves voted for the best poster(s).

The Covid-19 pandemic delayed our in-person meeting. However, this gave us a chance to hold a virtual get-together event a year before, which was organized in a brainstorming format and encouraged people to register to the physical meeting. The virtual meeting inspired six emergent topics that we formulated to one-hour discussion groups during the workshop to specifically address those issues. These discussion sessions were ignited by panels of invited speakers and actively attended by all participants, and actively involved the junior attendees. These sessions became the key-point for the synergetic mix of interdisciplinary opinions to unleash itself in an informal discussion and transported this spirit to the talks, where the speakers frequently made links to the topics discussed in the respective discussion groups. Importantly those sessions helped "experienced" newcomers (from other fields) to integrate, as well as "junior" newcomers to feel the general vibe of the topic and get involved and contributing ideas.

Overall, the atmosphere of the meeting was a non-stop dynamic and multimodal discussion, which we believe will lead to a number of concrete scientific results and cross-continental collaborations between experienced scientists and students arriving from the USA, Europe, Israel, and India. Dedicated to the topic of our meeting, there will be a special issue of the Journal of Bacteriology to which all the speakers and poster presenters were invited to contribute. That also provides an option for the scientific organizers to provide a perspective view based on the conference discussions. Several emerging collaborations between participants were apparent from the interactions. Furthermore, the recently started DFG Priority Program "Emergent Functions of Bacterial Multicellularity" (speaker T. Mascher) was introduced to the international community and should further increase the interdisciplinary and coordinated activities on

biofilm form of microbial existence. Undoubtedly, this event is just the first one in the series of the workshops to follow in the future.

Physical Biology Circle Meeting
Focus Workshop
Scientific coordinators: F. Jülicher, P. Haas, S. Rulands

The Physical Biology Circle Meeting is an annual series of meetings bringing together researchers in experimental and theoretical biological physics from its node institutions throughout Europe. Current nodes include, among others, mpi**pks** in Dresden, Institut Curie in Paris, EMBL Heidelberg, IST Austria, IBEC Barcelona, and the newest node, the Gulbenkian Institute in Lisbon. The 2023 meeting in Dresden gathered 87 on-site participants and 45 virtual participants who attended the talks via zoom.

The scientific focus of the Circle Meeting is broad, with contributions ranging from tissue mechanics to stochastic thermodynamics and from phase separation to cell signalling physics. Two keynote talks were presented by Otger Campàs and Maximina Yun from TU Dresden who spoke, respectively, about the multiple role of mechanics in morphogenesis and the biophysics of regeneration and ageing in salamanders.

The main emphasis was, however, on the active participation of postdocs and PhD students, who presented the contributed talks of 20 minutes duration, which were followed by lively discussions. Poster sessions in the evenings concluded the scientific programme.

After the fully hybrid Circle Meeting in 2021 (also hosted at mpi**pks**), we were very happy to be able to offer a "semi-hybrid format", with all speakers and poster presenters on-site, but some virtual attendance at the talks (which enabled those participants whom we had to reject due to space limitatons to attend the meeting).

This Physical Biology Meeting, the largest meeting organised at mpi**pks** since the start of the pandemic, enabled early-career researchs from the key European bophysics institutions to get to know each other and each others' work, which we are confident will lead to future collaborations.

New Perspectives in Active Systems
Workshop
Scientific coordinators: C. Huepe, F. Peruani

The workshop "New perspectives in Active Systems", organized by scientific coordinators Fernando Peruani and Cristián Huepe, took place at the Max-Planck Institute for the Physics of Complex Systems (mpi**pks**) in Dresden, April 24–28, 2023. The meeting was a great success, gathering over 200 participants from all over the world, including 60 on-site and almost 150 online. To develop a community-building experience, and maximize interactions, all presenters were required to attend in person.

The goal of the meeting was to go beyond standard descriptions of active systems by discussing models and experiments that explore new types of dynamics, interactions, and emergent states. To this end, we brought together researchers working on experiments, simulations, data analysis, and theoretical concepts that we expect to become increasingly central to the field in the next few years. To set the tone of the workshop, both scientific coordinators delivered a joint colloquium that highlighted the many new interesting research directions that are yet to be explored in active systems and their relevance for understanding the self-organization of natural and artificial systems at multiple scales.

Among the invited speakers, G. de Polavieja (Champalimaud Foundation) and G. Theraulaz (CNRS Toulouse) described new ways to extract the interactions in animal groups from tracking datasets. P. Romanczuk (Humboldt U. Berlin) discussed evidence of criticality in animal collective behavior. O. Dauchot (ESPCI Paris), S. Henkes (Leiden U.), and Y. Wu (The Chinese U. of Hong Kong) presented experiments and theory in the emerging field of active elastic dense and solid systems. D. Hu (Georgia Inst. of Tech.) and A. Perna (U. of Roehampton London) showed different physical structures that can emerge in insect collectives. G. Ariel (Bar Ilan U.) and D. Chaudhuri (Inst. of Phys., Bhubaneswar) introduced statistical mechanics extensions to active systems. E. Frey (LMU München) discussed novel nonequilibrium active matter states. Finally, J.-F. Joanny (Collège de France) presented a description of active turbulence, E. Lushi (New Jersey Inst. of Tech.) detailed new simulation approaches, and M. Turner (U. of Warwick) introduced a system of active particles equipped with artificial intelligence.

These topics were complemented with over 20 selected contributed talks. These presentations greatly enhanced the scope of the meeting and included many experts in the field as well as early career researchers. Additionally, approximately 20 posters were presented in a lively poster session.

One of the highlights of the workshop was an organized group brainstorming activity during a two-and-a-half-hour slot on Thursday. In this activity, we invited all participants to answer the question: "which should be the hot research topics in active systems in 10 years?" The group was divided into four breakout rooms, each for a different research area or approach: biological systems, artificial systems, modelling, and theory. We then gathered back in the main room and each group moderator presented the ideas that were discussed. The activity was highly successful, fostering vibrant discussions and an interesting confluence of perspectives. Most workshop participants took part in the conversations and expressed their appreciation for an exercise that invited them to think beyond their day-to-day research questions and allowed them to interact in new ways with their colleagues.

The workshop organization was handled flawlessly by the Visitors Program, initially by Maria Voigt and then by Claudia Domaschke. Both did a fantastic job, managing the many administrative demands of the meeting as well as multiple requests from the participants.

In sum, the workshop was extremely successful in helping develop new collaborations and perspectives in the very interdisciplinary field of active systems, as expressed to us directly by many participants, especially early career researchers. We believe it will lead to new research ideas and collaborative efforts and look forward to the possibility of organizing a similar event in future years.

Dynamical Control of Quantum Materials
Workshop
Scientific coordinators: D. Kennes, J. McIver, M. Sentef

The workshop "Dynamical Control of Quantum Materials", organized at the Max Planck Institute for the Physics of Complex Systems (mpi**pks**), brought together the emergent community of researchers working towards utilizing ultrafast light-matter interactions to achieve targeted many-body and topological states and novel functionalities in modern quantum materials. This event was a tremendous success and could not have happened without the dedicated commitment and highly professional organization by Mandy Lochar and the fantastic technical support by Ronny Börner.

More than 70 participants from diverse backgrounds enjoyed exciting and inspiring presentations by leading researchers and rising stars in the field. Topics covered included novel paradigms for photoinduced phase transitions, terahertz and lightwave control of electronic and lattice degrees of freedom, Floquet topology in cold atoms and topological edge modes in photonic crystals, Higgs spectroscopy in driven superconductors, designer metastable states and nonthermal pathways towards ultrafast control, Floquet states at the boundary of space and time resolution, novel probes of microscopic dynamics and collective excitations, cavity quantum materials, and new theory directions potentially guiding future experiments.

We witnessed an inspiring colloquium talk by Matteo Mitrano from Harvard University who presented the vision of connecting quantum information concepts and multipartite entanglement dynamics with scattering probes of condensed matter.

In total 24 invited talks and 13 contributed talks reported both on recent and partially unpublished experimental progress at the forefront of the field and on new theoretical ideas. On top of that, we had two very interactive poster sessions with around 40 posters, kicked off by plenary sessions with 2-minute flash talks where young researchers had the opportunity to advertise their work and posters to the audience.

The social event on Wednesday afternoon with the excursion to Moritzburg Castle and a wonderful conference dinner completed an inspiring workshop week.

We are extremely happy with how the workshop played out, and are happy to report that we received overwhelming and exclusively positive feedback by both more experienced and young participants. Comments include "I cannot remember being at an event where there were simply no boring talks", "Fantastic workshop – I am going back to work on my PhD thesis invigorated and inspired with so many new ideas", "I finally met all of these great researchers in person that I only knew from reading their papers", "I made so many new friends thanks to the relaxed and stimulating atmosphere at this fantastic workshop".

We can only add to this that the venue at mpi**pks** played an important role in making this workshop a big success.

Decomposing Multivariate Information in Complex Systems
Workshop
Scientific coordinators: C. Finn, A. Pakman, M. Wibr

The main focus of the conference was on partial information decomposition (PID), a recent extension of information theory that seeks to partition the total information provided by a set of sources into its unique, redundant and synergistic components, a task that is not addressed by Shannon's information theory. Due to the nascent state of PID theory, important theoretical work is ongoing and the conference proved very important to bring the field forward in this regard.

The question addressed by PID, however, is ubiquitous in many branches of natural sciences, and the conference thus covered also a range of early practical applications of PID theory, especially from the fields of machine learning and neuroscience. Here, the workshop format proved valuable to the participants as recent advances in PID theory helped to interpret these early empirical findings much more precisely.

In a field like PID that is still very much in flux, every participant is important, and often essential contributions are made by outsiders and newcomers. Thus, it is somewhat difficult to name the most important participants. Historically, however, the first insights into the PID problem were obtained roughly a decade ago by Randall Beer, University of Indiana, Bloomington, whom we could win to give a keynote lecture on how the ideas leading to PID were conceived. Certain other participants can be considered important due to their established status in fields related to PID, such as applied mathematics, represented by Jürgen Jost (MPI Mathematics in the Sciences), artificial intelligence, represented by Daniel Polani (University of Hartfordshire) and Greg ver Steg (Caltech), complex systems and information geometry, represented by Nihat Ay (Santa Fe Institute and Hamburg University), and information theory in neuroscience, represented by Stefano Panzeri (Italian Institute of Technology and Hamburg University).

However, in a young field often the newcomers make important contributions. The newcomers were fully integrated into the workshop track, i.e. we made little to no difference between presentations slots for newcomers versus established researchers. Several newcomers indeed made important contributions. Most of them may be a bit too technical for the scope of this report, but to give an example Aaron Gutknecht presented a unifying framework which formally explained why multiple approaches to the PID problem exist and that all of these approaches can be neatly organized into just 4 families – immediately rendering the field of PID much less confusing and more accessible.

Aaron Gutknecht's organization scheme encompassing and systematically relating the different PID approaches was also one of the main scientific results. The other important result arose from a discussion around the presentation of Artemy Kolchinsky, who showed that PIDs not respecting the set-theoretic inclusion-exclusion principle should be considered. In the course of the ensuing discussion it turned out that approaches to PID may be sorted into: (A) approaches that require the union information to be a random variable –enabling the use of information channels and the Blackwell ordering on channels, but often conflicting with the inclusion exclusion principle–, and (B) approaches honoring the inclusion-exclusion principle, but potentially sacrificing the representation of the parts of a PID a (auxiliary) random variables.

Overall, participants really enjoyed the workshop very much, not least because larger meetings on this topics have been rare in the past – despite of the rapid gain in attention that the field of PID gets. Therefore, the organizers and the participants would like to thank the Max Planck Institute for the Physics of Complex Systems again for the amazing opportunity to hold this meeting in Dresden, and to stress the importance of this support for them.

Active Matter at Surfaces and in Complex Environments
Workshop
Scientific coordinators: M. Tasinkevich, M. Telo da Gama, W. Uspal

Aim and focus. Active matter represents a new class of non-equilibrium soft condensed matter where energy extraction and consumption take place at the level of individual microscopic constituents. Examples include unicellular microorganisms and synthetic active colloids. This workshop was organized in response to the growing interest concerning active matter in complex and inhomogeneous environments. Here, the notion of "complex" applies to either the geometric confinement, the fluid host medium, or the combination of both. The interest in complexity arises from at least two directions: challenges in applications (for instance, bio-fluid viscoelasticity, ambient flows, and fluid/solid interfaces are ubiquitous

in vivo), and as a new means to control active matter systems (e.g., with chemically and topographically patterned interfaces). Thus, specific topics considered including confined active nematics, synthetic active colloids at interfaces, biological microswimmers in complex fluids and porous media, and microrheology of active suspensions. The underlying common feature in all these examples is that a wealth of length and time scales are introduced by the hierarchical structures of the environment and by the intrinsic structure and dynamics of the active fluids under consideration. Understanding these phenomena requires highly innovative approaches, which synergistically combine experimental, theoretical, and computational tools. Therefore, the organizers sought to balance the program between these three areas. Moreover, age, gender and geographical diversity were given explicit consideration in selection of talks. Out of thirty-nine talks, six were given by female researchers, and six by junior researchers (Ph.D. students, postdocs, and assistant professors / junior group leaders). The conference had participation from the EU, the USA, the UK, Canada, India, China, Singapore, Chile, and Brazil.

Most important participants. Since many leading researchers participated in the workshop as invited speakers, it is difficult to single out specific contributions. However, the workshop revealed some emerging directions in active matter, which can be connected with individual senior speakers. These emerging directions include perception/cognition and sensorial delay (C. Bechinger, G. Gompper), active unjamming (M. Dijkstra), and patterned motility landscapes (H. Stark, R. DiLeonardo). One highlight was the colloquium address, delivered by Jacques Prost. This talk provided a tour of seminal developments in cell motility and tissue dynamics, culminating in today's open scientific questions.

Newcomers. The talks and posters from junior researchers were of high quality. It was clarifying to have some important recent articles and pre-prints explained by their first authors. Some specific examples include the talks on "entropons," a newly identified class of non-equilibrium collective excitations (L. Caprini); motility and scission of an active fluid droplet on a planar surface (R. Coelho); and flows driven by interfacially active "carpets" (F. Guzmán-Lastra). Several junior researchers commented on the positive career implications of networking with senior researchers, e.g., for securing referee letters for tenure/promotion, or for obtaining postdoctoral positions.

Scientific results in the broader sense. The workshop achieved lively discussion after the talks and in poster sessions. Each talk stimulated at least several questions from the audience, with continued discussion frequently deferred to coffee breaks to keep the program on track. Several participants observed that the program of talks achieved a good balance between theory and experiment, and between various topics in active matter. It was also noted that the meals offered ample time for discussion. According to one of the mpi**pks** staff, there was excellent mixing and networking between participants in the coffee breaks. Expected outcomes of the conference include development of new research collaborations and cross-fertilization of ideas between different subareas of active matter. The workshop also underscored the need for enhanced communication and collaboration between experimentalists, computationalists, and theorists, given the intrinsic complexity and multiscale character of the systems under consideration. Scientific discussions initiated at this workshop are likely to continue at future meetings.

Control of Ultrafast (Attosecond and Strong Field) Processes Using Structured Light
Seminar and Focus Workshop
Scientific coordinators: C. Hernández-Garcia, M. Ivanov

Attosecond and strong field physics are evolving rapidly in several new directions, unified by the concept of lightwave electronics: the sub-femtosecond imaging and control of the electronic response of matter, from atoms to chiral molecules to quantum solids, using laser light structured in time and space to induce and resolve the desired dynamics. In parallel, new theoretical models and approximations are required to tackle these exciting as well as complex ultrafast dynamics. Therefore, the aim of the meeting was to bring together scientists from these three different and rarely interacting communities:

- structured light,
- attosecond and strong-field physics, and
- quantum solid state materials,

providing enough time for fostering their interaction and laying the foundation for developing collaborations between them.

With this goal in mind, the meeting included a 3-week long symposium and a 3-day long focus workshop. The symposium was aimed at theorists, with two 1.5-hour time slots for two talks per day in the morning and a free discussion time in the afternoon.

The 3-week period has given the participants enough time to interact with each other in a meaningful way, without time pressure and limits typical for discussions during conventional conferences. The focus workshop aimed at bringing representatives from the key experimental groups, providing the complementary perspective and the needed balance between the dreams of theorists and the realities of experimental labs.

The meeting was originally planned for the summer of 2020, but the pandemic forced several postponements, from 2020 to 2021, and from 2021 to 2023, when it was finally held in person. Given the goals of the event, an on-line format was impossible: a day-to-day human interaction was key to its success. The uncertainties with scheduling the event have led to several cancellations, but in the end, the meeting has attracted 66 participants from 17 countries.

Regarding the longer seminar aimed at theoreticians, these included highly visible scientists such as Prof. A. Landsman (Ohio State U, US), Prof. O. Smirnova (MBI, Germany), Prof. M. A. Porras (TU Madrid, Spain), Prof. Y. Murakami (RIKEN, Japan), Prof. K. Ishikawa (U of Tokyo, Japan), Prof. K. Krajewska (U Warsaw, Poland), Prof. X-B Bian (CAS, China), Prof. L. Plaja (U of Salamanca, Spain), Prof. A. Picon (U Autonoma Madrid, Spain), Prof. D. Milosevic (U Sarajevo, Bosnia and Herzegovina), Prof. L-Y Peng (U Peking, China), Prof. Kush Saha (NISER Bhubaneswar, India), Dr. S. Patchkovskii (MBI, Germany). They were joined by younger but already well-established scientists such as Prof. J-M Ngoko Djokap (U Nebraska, US), Dr. Maria Richter (MBI, Germany), Drs. E. Pisanty and M. Khokhlova (King's College London, UK), Dr. D. Ayuso (Imperial College/ Queen Mary College, London, UK), Drs. R.E.F. Silva and A. Jimenez-Galan (Materials Science Institute of Madrid, Spain), Dr. U. Bhattacharya (ICFO, Spain).

The workshop welcomed many very promising "scientific newcomers", such as Dr. Hao Liang (Peking U, China, and mpi**pks**, Germany), Dr. A. Ordonez (ICFO, Spain, and Imperial College London, UK), Dr. N. Mayer (MBI, Germany), R. Martin-Hernandez (U Salamanca, Spain), N. Rana (IIT Bombay, India), Dr. G. Brown (MBI, Germany), M. Even Tsur (Technion, Israel), and E. Bernal Molinero (Materials Science Institute of Madrid, Spain).

During the focus workshop, the symposium participants were joined by prominent scientists, such as Prof. O. Cohen (Technion, Israel), Prof. J. Burgdoerfer (TU Wien, Austria), Prof. J. Biegert (ICFO, Spain), Prof. T. Morishita (U of Electro-Communications, Japan), Prof. M. Lein (U Hannover, Germany), Prof. Th. Fennel (U Rostock, Germany), Prof. J. Berkadar (U Halle, Germany), Prof. T. Popmintchev (U California San Diego, US), Prof. S. Witte (ARCNL, The Netherlands), Prof. I. Fabrikant (U Nebraska, US), Prof. T. Ruchon (U. Paris-Saclay, France), Prof. F. Mauger (U Louisiana, US), Prof. G. Paulus (U Jena, Germany), Prof. C. Trallero (U Connecticut, US), Prof. M. Wollenhaupt (U Oldenburg, Germany), to name but a few.

The symposium participants were unanimous regarding the high quality of talks, with the unhurried pace of the symposium stimulating detailed and productive discussions. Importantly, all symposium participants spent significant time at the event, ensuring not only very lively discussions during the talks and in the afternoon, but also the emergence of new collaborations during the meeting, e.g. between Dr. M. Khokhlova (Kings College London) and the group of Prof. G. Dixit (IIT Bombay); Prof. O. Smirnova (MBI) and M. Even Tsur (Technion); Dr. U. Bhattacharya (ICFO) and Prof. M. Ivanov (MBI); Prof. Kush Saha (NISER Bhubaneswar) and Prof. M. Ivanov (MBI); Prof. L-Y. Peng , Dr. Hao Liang and Prof. O. Smirnova; Prof. S. Witte (ARCNL) and Prof. C. Hernandez-Garcia (U Salamanca); Prof. Picon (UAM), Prof. L. Plaja (U Salamanca) and Drs. R.E.F. Silva and A. Jimenez-Galan (Materials Science Institute of Madrid, Spain); Prof. M. A. Porras (TU Madrid) and Prof. C. Hernandez-Garcia (U Salamanca), among others.

The key scientific questions debated during these discussions were ultrafast nonlinear spectroscopy of topological and strongly correlated solids, applications of structured light for (i) generation and detection of ultrashort bursts of XUV light and of very strong magnetic fields, (ii) generation of electron vortices in photo-ionization, and (iii) generation and detection of ultrafast, enantio-sensitive electron currents in chiral molecules.

Some of the new ideas that have emerged during the workshop include the use of nonlinear optical response for probing topology of Fermi surfaces, the use of ultrafast light's topology to unveil electron correlation dynamics in solids, the use of artificial intelligence to boost strong-field calculations, and the development of new measures of chirality for applications in photo-electron spectroscopy of chiral matter.

The original vision for this meeting was championed by Prof. A. Starace, who has unfortunately passed away before the meeting took place. A memorial session in his honour, open to the public, has been held during the meeting. The session was held in the mixed format, with both in-person and on-line presentations, which gave the opportunity to friends, colleagues and family of Tony to take part. Tony has been instrumental for all aspects of the meeting, and his outstanding skills in identifying important topics and bringing people together will always be missed.

Elastic Manipulation and Dynamics of Quantum Materials
Seminar and Workshop
Scientific coordinators: J. Schmalian, J. Sinova, R. Valenti

The workshop and seminar Elastic Manipulation and Dynamics of Quantum Materials, held at the Max Planck Institute for the Physics of Complex Systems (mpi**pks**), marked an essential gathering of researchers in this vibrant field of hard condensed matter research. Their focus: to advance our understanding of physical phenomena that are the result of a strong coupling between electronic quantum orders and the crystalline lattice, over a wide range of time and length scales. This event achieved resounding success, a testament to the unwavering dedication and superb organization led by Mandy Lochar.

Over 80 participants from diverse backgrounds listened to captivating and enlightening presentations by renowned experts and emerging talents in the field. It was the nucleus for numerous discussions that included researchers from all generations.

Topics covered spanned spectroscopy of strain-tuned quantum materials (Bernhard Keimer, Marie-Aude Measson, Thais Trevisan, Michaela Souliou, Olena Fedchenko), the physics of driven systems (Andrea Cavalleri, Sangeeta Sharma, Peter Oppeneer, Premala Chandra), as well as states of complex order and superconductivity (Abhay Pasupathy, Rafael Fernandes, Clifford Hicks, Erez Berg, Andrey Chubukov, Sananda Biswas, Malte Grosche) and prospective theoretical directions guiding future experiments (Piers Coleman, Alex Levchenko, Francesco Ferrari). A significant number of these speakers were postdocs who impressed with wonderful and inspiring talks. Particular highlights of the event were the beautiful talks by Hilary Noad and Elena Gati and, last but not least, by Grgur Palle, who is a PhD student. A particularly inspiring moment transpired during a colloquium talk by Paul Canfield from the Ames Laboratory and Iowa State University, who unveiled his vision on the design and discovery of new correlated electron systems.

The workshop featured 23 invited talks and 11 contributed talks, shedding light on recent experimental advancements, some of which were disclosed for the first time, and pioneering theoretical concepts. Two highly interactive poster sessions accompanied by plenary sessions with concise 1-minute flash talks provided a platform for young researchers to showcase their work and engage with the audience.

We are thrilled with the workshop's resounding success and are pleased to report overwhelming and exclusively positive feedback from both seasoned experts and emerging researchers. Comments such as "this was the top workshop of the year for me...", "A great workshop – it boosted my enthusiasm of my ongoing PhD thesis work," and "Thanks to the mpi**pks** for this outstanding facility" resonate deeply.

Non-Hermitian Topology: from Classical Optics to Quantum Matter
Workshop
Scientific coordinators: E. J. Bergholtz, F. Piazza, J. C. Budich

The main objective and focus of the workshop was to catalyze the interdisciplinary exchange between various fields in the physical sciences on the timely topic of non-Hermitian topology. While non-Hermitian degeneracies, also known as exceptional points, and their topological properties have been discussed for many years in the (classical) optics community, the quantum-condensed-matter-driven subject of topological phases such as topological insulators and superconductors has only more recently been extended towards non-Hermitian physics to account for dissipative processes of various origin. In this light, to the knowledge of the organizers, this workshop was the first globally visible larger event which brought together leading experts with a broad range of backgrounds constituting a strong line-up of invited speakers.

Scientific presentations by newcomers were given high priority in at least two ways: First, the arguably most visible slots in the late morning session right before lunch were reserved for contributed talks, the majority of which was given by young scientists, several of which presented fresh and innovative approaches to the topic of non-Hermitian topology. Among these, the organisers would like to mention the

contribution of Ms. Janet Zhong (Stanford), who as a young graduate student and thus true newcomer really gave an impressive talk on Friday morning, where she even modified parts of her presentation over night (involving substantial simulations and new plots) to include the methodology presented by David Luitz on Thursday in her numerical analysis.

Second, the two poster sessions were not shifted to the late evening after dinner but took place in the afternoon which led to very high attendance.

From the overwhelmingly positive feedback by many participants as well as numerous inquiries regarding follow up conferences, the organizers are confident that this event has made a substantial contribution to transferring knowledge on the subject of non-Hermitian topology between otherwise scarcely communicating communities. This has led to the identification of possible new directions and experimental platforms.

Extreme Waves, Workshop
Scientific coordinators: N. Akhmediev, H. Brand, A. Chabchoub

The main focus of the workshop as expressed in its title is extreme waves in various physical media. These include extreme waves in the open ocean, experimental water facilities, and optical fibers. Extreme events in nature by now are well known and happen frequently in all parts of the globe. These include bushfires, floods, tornadoes, earthquakes, and tsunamis. Their frequency is visibly and noticeably increasing in recent years. Extreme waves are part of these phenomena that can be studied with relatively high precision. Moreover, they can be modeled theoretically using mathematical tools and reproduced experimentally in the lab. The possibility of common description of extreme waves in such different scales as optics and ocean waves allows interdisciplinary communication between scientists that otherwise would work separately without using the knowledge achieved in other areas.

Leading experts on these subjects present at the workshop included:

Prof. Norbert Hoffmann from Hamburg University of Technology (Germany), Prof. Joachim Peinke from Carl von Ossietzky University of Oldenburg (Germany), Prof. Majid Taki from the University of Lille (France), Prof. Matthias Fink from ESPCI Paris (France), Prof. Orazio Descalzi from the University of Andes (Chile), Prof. Cristina Masoller from the Polytechnic University of Catalonia (Spain), Dr. Matteo Conforti from the University of Lille (France), Prof. Goery Genty from Tampere University (Finland), Prof. Arnaud Mussot from the University of Lille (France), Prof. Fabio Baronio from the University of Brescia (Italy), Prof. Victor Shrira from Keele University (UK), Prof. Paolo Santini from the Sapienza University of Rome (Italy), Prof. Mustapha Tlidi from the Free University of Brussels (Belgium), Dr. Maura Brunetti from the University of Geneva (Switzerland), Dr. Margarida Facao from the University of Aveiro (Portugal), Prof. Thomas Adcock from the University of Oxford (UK), Prof. Uwe Bandelow from WIAS, Berlin (Germany), Prof. Wonkeun Chang from Nanyang Technological University (Singapore), Prof. Michelle Sander from Boston University (USA), Prof. Brian Haus from the University of Miami (USA), Prof. Stefan Wabnitz from the Sapienza University of Rome (Italy), Prof. Takuji Waseda from the University of Tokyo (Japan), Prof. Holger Kantz, mpi**pks**, Dresden (Germany).

Among the newcomers to the field and the young researchers who made visible contributions to the state of the research area we mention:

Prof. Yan Li from the University of Bergen (Norway), Dr. Ioannis Karmpadakis from Imperial College London (UK), Dr. Alberto Alberello from the University of East Anglia (UK), Dr. Raphael Stuhlmeier from the University of Plymouth (UK), Mr. Maxime Canard a Master student from Ecole Centrale de Nantes (France), Dr. Ludovica Dieli from the Sapienza University of Rome (Italy), Ms. Tatiana Tarasova from Passau University (Germany), Dr. Andrei Gelash from the University of Burgundy (France).

An important part of extreme wave research is its practical applications. First, let us mention the novel directions that appeared in recent years. The role of ice on the surface of water in generation of extreme waves, spectral downshift of waves and the wave dissipation has been considered in a few talks. As significant areas of the world ocean are covered by ice, this research reveals the specific dynamics of waves in such areas. Counter-propagating waves and their influence on extreme wave dynamics is another area considered at the workshop. This is relevant to the so-called crossing seas when the waves are propagating in all directions of the two-dimensional ocean surface. Extreme weather events have been discussed by Prof. Kantz. He used daily precipitation data and water levels of the river Elbe for the illustration of extremes. These can be further extended to illustrate weather changes due to climate change.

Modulation instability (MI) is at the root of spontaneous appearance of extreme waves, as has been confirmed in the majorities of the talks given. Despite many years of research efforts, MI remains a complex phenomenon that is at the center of attention of many researchers. The number of publications on this subject has increased exponentially over the last few years. Significant attention to this subject has also been paid at the workshop. Its tight relation to Akhmediev breathers is one of the major points that reveals the long-term evolution of MI. Recent discoveries include the wider range of frequencies that lead to MI.

A deeper look into the mathematical concepts of rogue waves has been given by Prof. Santini. Using the theory developed for the NLSE, he extended it to the case of 2+1 dimensions covering Davey-Stewartson II equation that is also integrable and admits exact solutions. Further extension of these results to the case of the KP equation have been presented in the talk by Prof. Maruno.

Statistical analysis is an important part of rogue wave studies. Multi-point statistical analysis and comparison of empirical data of waves in turbulent state has been presented by Prof. Peinke. An interesting point of his analysis is that the extreme waves are associated with negative entropy. This conclusion could be one of the fundamental results that may have far-reaching consequences. A statistical approach based on kinetic equations has been presented by Ms. Tarasova. The latter can be applied to a large variety of media where extreme waves appear in the form of multi-soliton gas in shallow water using the Korteweg-de Vries formalism. Experimental statistical data on extreme waves in a 150 m water tank have been presented by Mr. Canard. These results provide links between the extreme crest distributions, the modulations of the wave envelope, and the nonlinearity of the system. Extreme wave statistics in the cases of intermediate and shallow water depths have been presented by Dr. Karmpadakis. These studies are based on both, sea surface measurements and the lab data. These experimental data can be used to create a predictive model for crest height statistics.

An important aspect of research on extreme waves is their prediction. Extreme waves that appear in ocean currents have been analyzed by Prof. Shrira. The ocean currents (like notorious Agulhas current in the Indian Ocean) allow for resonant triad interactions that do not exist without the current. One of the interacting waves becomes longer and may serve as a precursor of an extreme wave. This possibility has been theoretically investigated.

Optical extreme waves have been presented in a number of talks. Quadratic optical media is one of the possibilities. Prof. Schiek addressed this issue in his experimental studies of Akhmediev breathers and modulation instability that essentially lead to extreme waves. These studies are done in spatial geometry that is a counterpart of the wave evolution in time. Prof. Baronio made further steps in this idea and investigated resonant radiation emitted by the Akhmediev breathers and the Peregine soliton that is a particular case of the Akhmediev breather at zero frequency. The studies of extreme waves in multi-mode fibers have been presented by Prof. Wabnitz. These are also related to the second-harmonic generation. Beam breaking into filaments revealed extreme local intensity peaks.

Last, but certainly not least, novel machine-learning techniques for ocean wave prediction for the purpose of operational prediction of rogue waves in the ocean have been reported by Prof. Hoffmann. These advances have a strong potential to be used on ships or fixed marine installations and could predict the formation of large-amplitude waves within a few minutes. It is also worthy to mention that for popularizing the subject Prof. Hoffmann presented a public lecture for the citizens of Dresden informing them about the extreme waves in nature and their most recent scientific studies. The lecture attracted a significant number of people interested in extremes.

It is hard to list all impactful talks made at the workshop. Overall, significant progress has been achieved in the area of extreme waves that have been amplified by additional three years of intensive research on the subject during the pandemics time. There is no doubt that this workshop will serve as one of the significant roadmaps in further progress in the quickly developing area of extreme waves, which appears to become a discipline of its own.

Korrelationstage 2023
Workshop
Scientific coordinators: I. Eremin, L. Fritz, M. Vergniory

The workshop took place at **mpipks** in Dresden on September 11 – September 15, 2023 and continued a long standing tradition in bringing together researchers mostly working in the field of strongly correlated (electronic) systems and related areas. The main focus of this event was to capture the new developments

in this active field, with a particular emphasis on the new realizations of the correlated quantum matter including but not limited to heterostructures of 2d materials as well as analytical and numerical methods development, which happened over the past several years. The format of the meeting was chosen such that there were only very few invited talks and most of the research talks, selected from the submitted contributions, were presented by junior (non-tenured) scientists. The poster presentations were solicited from everybody.

The workshop covered a range of topics, including the novel development in the field of non-trivial topology in correlated and magnetic systems, interplay of topology and superconductivity, recent advances in the numerical methods like DMRG and quantum Monte Carlo, and development of new algorithms for the quantum computer. During the workshop a number of phenomenological and microscopic theories have been discussed in informal but serious manner. In addition this workshop promoted scientific exchange and interaction between researchers working in these and related areas.

Over 90 participants from Europe, Asia, and USA took part in the meeting. The program included 40 oral presentations, both invited and contributed, as well as two poster sessions with overall 54 posters. The interchange of points of view between participants with distinct scientific interests gave rise to a highly stimulating atmosphere. During the workshop a number of new and exciting results have been presented by, e.g., Frank Schindler (Imperial College London) on "Nonlinear breathers in obstructed atomic bands", Johannes Knolle (Technische Universität München) on "Anomalous quantum oscillations in metals and insulators", Jonah Waissman (The Hebrew University of Jerusalem) on "Detecting emergent magnons in graphene via thermal transport", Natalia Chepiga (TU Delft) on "Resilient infinite randomness criticality for a disordered chain of interacting Majorana fermions", and Mathias Scheurer (University of Stuttgart) on "Exotic many-body physics in van der Waals moiré systems". Many other, especially young, participants presented talks of high quality and showed new and interesting results. The talks, discussions, and posters at Korrelationstage 2023 demonstrated that the field of correlated electrons is developing rapidly and has great prospects.

Two main results of the Workshop are (i) a focused exchange of ideas on the recent theoretical developments in the field of strongly correlated electrons and related systems and (ii) an involvement of young scientists in the discussion which has stimulated new research collaborations.

We would like to thank mpi**pks** for its hospitality and excellent infrastructure provided to the participants of the workshop. We also would like to thank the team of secretaries and, in particular, Katrin Lantsch for their kind assistance and excellent support of this meeting.

Quantum Materials in the Quantum Information Era
Workshop
Scientific coordinators: J. Checkelsky, Q. Si, R. Valenti

The international workshop QMATQI23 took place from September 25 – 29, 2023. There were 72 participants from 13 countries. The aim of the workshop was to bring together scientists working in various aspects of quantum materials with potential relevance to quantum information, highlighting the progress and prospects for advancement in this emerging area.

The workshop included speakers from various sub-areas and included both theory and experiment. For example, in the area of quantum magnetism Alan Tennant delivered a lecture on entanglement in quantum magnets and its measurement and Hae-Young Kee a lecture on theoretical developments in multipolar spin liquids. In the area of 2D systems, lectures included those by Mitali Banerjee on thermal signatures of edge states in quantum Hall systems and by Ady Stern on proposed approaches for using electronic conductance to probe anyonic statistics. In the area of novel topological electronic systems, examples were Nandini Trivedi with a lecture on using orbital frustration to design topological flat bands and Yoshi Maeno on recent updates on the strontium ruthenate superconductor. We held two discussion sessions, wherein topics and questions were submitted by audience members using an online system as well as in hand-written form. The audience responded to these questions, proposing ideas and concepts in interactive sessions.

In addition to the above activities, there were aspects targeted specifically for junior scientist participation. This included two poster presentation sessions with two associated short poster talk sessions. In the latter, junior participants gave two-minute presentations about their posters. Several junior participants and other contributing participants were also selected to deliver contributed talks along with the invited speakers.

The workshop activities identified several key areas for the consideration of the future development of this research area:

- Are there problems from the quantum materials realm that could be profitably addressed with quantum devices?
- How can topology be best used for quantum information?
- What quantum information quantity would characterize quantum criticality?

The organizers noticed a distinct cross-fertilization between the scientific sub-areas as the workshop proceeded. It was clear that some concepts developed in e.g. quantum magnetism in the context of entanglement witnesses could be used to extend considerations in low-dimensional systems. It is expected that this will help to germinate new ideas in the future for connecting quantum information and quantum materials.

The organizers express their sincere thanks to the Max Planck Institute for the Physics of Complex Systems for hosting us, to the Institute staff for their expert support in running this workshop. Particular thanks are expressed to Mandy Lochar for excellent organizational support and Ronny Börner for impeccable technical support with the sessions.

Non-autonomous Dynamics in Complex Systems: Theory and Applications to Critical Transitions
Seminar and Workshop
Scientific coordinators: P. Ashwin, U. Feudel, M. Ghil

According to the goal of this workshop/seminar we brought together scientists from various disciplines in the natural sciences, such as mathematics, physics, the climate sciences, neuroscience, ecology, systems biology, and network science. Almost all speakers who have been invited accepted our invitation, so that most of the major players in this field were present in the workshop. Therefore, this workshop was very attractive for people in the above areas. Overall, we had at the workshop 90 participants from 21 countries spread over Europe, Asia, North and South America as well as from Australia. Since this workshop was planned as an on-site event almost all speakers were in person in Dresden, except for one speaker from China, who did not get the visa for Germany in time and one speaker from Israel, who could not leave because of the Gaza conflict. Both invited speakers gave their talks online. In addition, we had another short-term cancellation due to entry problems at the border and we filled this slot with another invited speaker, who could not make it to Dresden on such short notice. All talks were recorded but only available for the participants using their password for the workshop.

Non-autonomous dynamics as the main theme of the workshop has been presented from a theoretical point of view featuring new mathematical methodology [A. von der Heydt (The Netherlands), C.K.R.T. Jones (USA), M. Rasmussen (UK), S. Wieczorek (Ireland)], and different applications in climate dynamics [T. Tél (Hungary)], ecology [E. Meron (Israel), P. Dutta (India)], neuroscience [K. Lehnertz (Germany)], medical science [L. Chen (China)], machine learning [P. Tino (UK), Juan-Pablo Ortega (Singapore)], socio-ecological systems [S. Roman (UK)] and astrophysics [T. Kovács (Hungary)]. Already this list highlights the interdisciplinarity of the event. Of particular interest for many applications were rate-induced transitions between the different stable states, a typical bifurcation in non-autonomous systems also called a tipping point. These bifurcations are caused by changes in the internal parameters of the system, changes in the forcing leading to a transition from one stable state to another when the rate of change is larger than a critical rate. Such transitions have been presented in several applications like the changes in the Atlantic overturning circulation [P. Ditlevsen (Denmark), H. Dijkstra (The Netherlands)], the melting of ice sheets [M. Montoya (Spain)], or changes in ecosystems [M. Silber (USA)] as a response to climate change. But also new theoretical ideas such as basin instabilities, the combination of rate-induced and noise-induced transitions as well as topological instabilities have been presented [G. Charó (Argentina)]. Besides theoretical investigations based on model systems, new approaches to identifying critical transitions from time series [N. Boers (Germany)] have been discussed. Overall, 22 invited talks and 23 contributed talks demonstrated the state-of-the-art in the field of non-autonomous dynamics in complex systems and facilitated very lively discussions leading to the intended cross-fertilization between the different fields.

Many of the participants were early career researchers. Therefore, we included 2 poster sessions, each one in the evening as an "open-ended" event after a short two-minute presentation of each poster by its presenter in the afternoon. The broad spectrum of topics in the talks was also reflected in these two

very busy poster sessions where early career researchers presented their results for an open discussion. All the posters were on a very high scientific level so that the poster judges, P. Ditlevsen (Denmark), C.K.R.T. Jones (USA), S. Pierini (Italy), M. Rasmussen (UK) and M. Silber (USA), had a hard time to select the very best ones for the 3 poster prices.

As a result of this workshop, we expect that several joint papers with different participants of the workshop will appear in the future. The organizers have arranged for a Focus Issue dedicated to this workshop in the international peer-reviewed journal CHAOS: An Interdisciplinary Journal of Nonlinear Science, with about 40 invited papers. This Focus Issue has already been advertised on the journal's website and it will appear, we hope and expect, in early 2025.

Overall, this workshop was a very successful event, bringing together scientists from various disciplines, which usually would not meet in their different disciplinary conferences. The organizers got a lot of positive feedback afterwards, encouraging us to organize another event of similar format at some later time. Since this field of research is still in its infancy but rapidly developing, organizing such a follow-up event in the coming years is sound advice.

One week before and after the workshop we organized a seminar, which had a school-like character with lectures given by C.R.K.T. Jones (USA), K. Lehnertz (Germany), E. Meron (Israel), M. Rasmussen (UK), D. Sciamarella (Argentina), and the three organizers. In addition, three short courses including hands-on parts were presented by I. Longo (UK) on "Critical transitions in non-autonomous systems", M. Ghil and D. Ohara on "Singular Spectrum Analysis", and G. Datseris (UK) on "Programing Language Julia and its Application in Dynamical System Theory". This program attracted many early career researchers. Thus, we had to make a very restrictive selection of the participants, since we had 44 applicants for only 25 places, including the places for the lecturers. We followed the rule that from each working group we only accepted one student or postdoc. To solve the problem which student/postdoc to choose from several applications in the same group, we communicated with the supervisors of the applicants. This way a group of 20 students coming from 17 distinct universities and scientific institutes was selected, supplemented by 4 local students, 3 from the Max-Planck-Institute for Physics of Complex Systems and 1 from the Max-Planck- Institute for Animal Behavior: overall, just 15 PhD students and 9 postdocs from 9 countries.

Fractional Quantum Anomalous Hall Effect and Fractional Chern Insulators
Workshop
Scientific coordinators: Z. Liu, J. van den Brink, Y. Zhang

The international workshop **FQAH24** took place from February 5 - 8, 2024. There were 76 participants from 16 countries. The aim of the workshop was to bring together scientists working in various aspects of the fractional quantum Hall effect and its experimental realization in engineered moiré materials, highlighting the progress and prospects for the recent experimental breakthrough on the quantized fractional Hall resistance at zero magnetic field.

The workshop included speakers from various sub-areas and covered both theory and experiment. For example, in the area of the fractional quantum anomalous Hall effect and moiré materials, Long Ju gave an opening lecture reviewing the recent development of realizing correlated and topological states in moiré systems, and presented his experimental work on the fractional quantum anomalous Hall effect in pentalayer-graphene. Xiaodong Xu gave a colloquium talk on his journey of realizing the fractional quantum anomalous Hall effect in twisted MoTe2, from the optical signature to the final evidence in transport experiments. Tingxin Li reported the observation of integer and fractional quantum anomalous Hall effects in 2D semiconductor moiré superlattices. Several speakers, for example Bogdan A. Bernevig, Kai Sun, and Nicolas Regnault, focused on the theory of fractional Chern insulators in moiré materials. Some talks, such as those by Andreas Läuchli, Steven H. Simon, and Oskar Vafek, discussed correlated phases beyond fractional Chern insulators in moiré materials. On the transport theory, examples were Sankar Das Sarma on analyzing quantum anomalous Hall effect experiments in the context of the conventional quantum Hall effect, and Ady Stern on composite Fermi liquids in half filled Chern bands. In the area of ab initio simulation of large scale systems, Jeil Jung and Jianpeng Liu talked about modelling of pentalayer-graphene, and Di Xiao and Ting Cao gave presentations on the machine learning force field applied to twisted WSe2 and MoTe2. There were also talks about the bosonic fractional quantum Hall effect, such as those from Ruirui Du on the bosonic Laughlin state in a moat band without magnetic field, and from Nathan Goldman on the strongly-correlated topological matter with quantum gases. In the closing remark, Emil Bergholtz listed several key open questions in the field of the fractional quantum

anomalous Hall effect and fractional Chern insulators, the breakthroughs on which are highly demanded. Overall, the talks in this workshop demonstrated the state-of-the-art in the field.

The contributions from young scientists are very important for the progress of the field. Several invited talks in this workshop were given by speakers who had recently obtained faculty positions, including Yonglong Xie, Trithep Devakul and Jie Wang. There were also two poster sessions on the first two days of the workshop. Thirty participants, most of whom are PhD students and postdocs, contributed poster presentations which led to high attendance. The organizers are happy to see that this workshop brought people working on the quantum Hall effect, two-dimensional materials, cold atoms, and ab initio simulation together and led to fruitful discussions. It was clear that the participants from different communities united under a common keen interest on the fractional quantum anomalous Hall effect and fractional Chern insulators. From the positive feedback by many participants, the organizers are confident that this event provided an excellent platform to exchange ideas, identify key scientific problems, and initiate collaborations, which will keep the research field flourish in the future.

Quantum Interactive Dynamics
Workshop
Scientific coordinators: R. Moessner, F. Pollmann, A. Smith, S. Sondhi

Quantum many-body systems out of equilibrium represent a challenging frontier and have been shown to exhibit extremely rich phenomena. Recent experimental advances in building Noisy Intermediate-Scale Quantum (NISQ) devices have opened up a completely new territory in this context. The natural evolution implemented by NISQ devices is a quantum interactive dynamics generated by a combination of unitary gates and measurements. These platforms provide an opportunity to explore vastly larger parts of the Hilbert space and go beyond what can be realized in purely unitary systems.

In pioneering works, an entanglement phase transition was identified in the dynamics of circuits of random unitary gates interleaved with local projective measurements. This phase transition separates a disentangling phase, obeying an area law, and an entangling phase obeying a volume law. Successively, it has been shown that additional phase transitions between different area phases can occur and new kinds of quantum phase transitions have been discovered.

The international workshop on **Quantum Interactive Dynamics** focussed on recent developments in this new field and brought together a small group of experts from academia and industry. The workshop was held in-person with one remote talk. The format included 18 invited talks spread across a two and a half day program and particularly focussed on the following topics:

- Noisy Intermediate-Scale Quantum (NISQ) devices [talks by Hannes Bernien (US), Xiao Mi (US), Hongzheng Zhao (CN)]
- Measurement based transitions [Tianci Zhou (US)]
- Open quantum systems [Vir Bulchandani (US)]
- Error correction [Sagar Vijay (US)]
- Computational complexity
- Classical shadows [Andreas Elben (US)]

Beyond those topics, additional themes emerged:

- Active phases of matter [Tibor Rakovszky (US)]
- Classically-assisted quantum state preparation [Barbara Kraus (DE), Henrik Dreyer (DE), Ruben Verresen (US), Kevin Smith (US), Marin Bukov (DE)]
- Tests of ergodicity [Samuel Garratt (US), Mari Carmen Bañuls (DE), Federica Maria Surace (US)]
- Constrained quantum dynamics [Katja Klobas (UK), Tomaž Prosen (SLO)]

The workshop brought together leading experts from the USA, China, UK, and Europe, and the invited talks of all sessions led to stimulating discussions. Given the high-quality contributions, which addressed all of the topics that were set out and beyond, we believe the goal of the workshop was clearly achieved.

Information processing, Noise, and Adaptation in Living Systems
Workshop
Scientific coordinators: N. Barkai, D. M. Busiello, C. Zechner

The main goal of the conference was to bring together different communities interested in the same broad questions on how living systems process information from the environment and consequently respond to it. The presence of renowned researchers from various fields, from engineering to statistical physics and biology, has been instrumental to successfully reach the expected aim. In particular, we had the colloquium talk by Yuhai Tu, one of the most known scientists in the field of information processing and biophysics, and a keynote talk by Andre Levchenko, director of the System Biology Center at Yale University, and several speakers from the USA (Prof. Ilya Nemenman, Prof. Andreas Hilfinger, Prof. Andrew Mugler, Prof. Matthieu Louis, just to mention a few). Despite the multitude of approaches that have been presented and the unavoidable modulations of the scientific language employed, each one of the talks was focused on a set of questions common to the entire audience. This made the workshop particularly interesting in its wholeness, with no over-specific or out-of-focus sessions. The feedback we received from the community were extremely positive about the possibility to follow every scientific session with interest, most importantly leaving open the possibility to be surprised by unknown methods – coming from different areas of science – to tackle similar problems.

We also left some open time slots to favor discussions among members of those communities involved. Indeed, discussions were fruitful and frequent so that more time dedicated to them would have been useful, according to several participants. Although we were not able to arrange additional slots for this scope, this feedback clearly suggests that the goal of the workshop has been reached, encouraging interdisciplinary discussions and collaborations on its subject. This lively and interactive environment also helped young scientists to know the community and meet more experienced researchers. We decided to select for posters mainly PhD students and young postdocs, so that they had plenty of time for detailed scientific discussions.

Overall, the workshop resulted in a stimulating environment where multiple communities interacted and exchanged ideas, in the spirit of the original scope of the event. Numerous and various approaches have been presented to similar questions, widening the perspective of experienced scientists and letting younger ones to know the field in a broader sense.

Interdisciplinary challenges in non-equilibrium physics: from soft to active, biological and complex matter
Workshop
Scientific coordinators: X. Chen, M. Rinaldin, A. Sciortino

Main focus of the conference. The IntCha workshop brought together novel ideas and expertise from various fields to address complex physical systems in an interdisciplinary manner, bridging the gaps between out-of-equilibrium physics and traditional soft matter, between theory and experiments, between simplified models and the intricacies of biological systems. Out-of-equilibrium physics in general aims at understanding a large variety of phenomena in systems that break time reversibility. This field is becoming more and more intertwined with different areas of Science thanks to its general nature and due to the ubiquity of non-equilibrium processes in biology, chemistry, and material science. This poses challenges and opportunities outside the traditional realms of Physics. In addition, as our experimental and theoretical tools improve, more and more complicated systems can now be effectively tackled. In the IntCha workshop, participants discussed how we can effectively bridge different fields to tackle interdisciplinary problems, how we deal with this complexity and how we train the next generation of scientists to cope with the increasingly interdisciplinary fields. The workshop offered an environment where young researchers with different, but connected, backgrounds exchanged their knowledge across different disciplines, at the boundary between different fields. Throughout five days, several talks from early career researchers, poster sessions, and Q&A sessions sparked discussions among participants, offered new interdisciplinary collaborations, and promoted the exchange of experiences and ideas.

Most important participants. Given the impressive contributions of 33 invited speakers and 50 poster presenters, it is challenging to emphasize individual contributions. The participants were very proactive and created a lively conference with energetic poster sessions and asked many questions after the talks. We would like to emphasise the scientific, geographical, and gender diversity of the participants. Among the participants, two thirds worked in theory and simulations and a third in experiments. Moreover, about

40% were female and about 60% male. The conference had participation from the EU, the USA, the UK, India, Philippines, Armenia, Japan, Republic of Korea, South Africa, China, Pakistan and Brazil. We would like to highlight the opening colloquium of Eleonora Secchi on bacterial biofilms which provided an outstanding example of the interplay between physics, biology, and material science. Another interesting contribution was the one of Agnese Curatolo and Elena Sesé-Sansa, editors at the American Physical Society. The editors gave a very useful overview of the scientific publishing process in general and at Physical Review Letter, Physical Review E and Physical Review X Life, three journals very important for the field of the conference. Their talk stimulated a participated discussion among the young researchers that continued during the Q&A session and lunches with the editors.

How did scientific newcomers present themselves? Aimed at early career researchers, IntCha24 offered scientific newcomers many ways of presenting themselves. Among the 33 speakers, three quarters were postdoctoral researchers who presented on diverse fields of interdisciplinary work. One fifth of the speakers were PhD students. Among the 110 participants, 50 scientific newcomers presented posters in the two poster sessions, including poster award-winning presentations by PhD candidate Y. Sarmiento on the interdisciplinary topic of human perceptual decision-making of non-equilibrium fluctuations, master student L. Schick on experiments of the decision-making process in light-trapped slime moulds, and PhD candidate F. de Luca on hyperuniformity in phase ordering. For the participants, IntCha24 has broadened the horizons of scientific newcomers. Among the 22 participants who have completed the feedback survey, 18 have gained unexpected interest in information in biology, while half have gained interest in topics such as cells and tissues, microorganisms, micro and nanofluids, and living polymers. Scientific newcomers also benefited from organized lunch discussions and presentations from editors of the American Physical Society (E. Sesé Sansa, A. Curatolo), where they found learning the editorial process very useful. Facilitated discussions on broad topics such as the impact of AI to science, publishing, and problems faced by early career researchers also brought out the voices of scientific newcomers. Finally, the workshop was shaped by the emergence of a community of early career researchers, whose enthusiasm and active participation were felt by both their peers and more senior attendees. This dynamic fostered a sense of community, encouraged potential collaborations, and helped reduce social barriers for others.

Scientific results of the conference in the broader sense. The workshop achieved several main results: it featured a broad range of topics in the field, allowing participants to get to know rising scientists in neighbouring domains and to acquire newfound interest on new issues; it cemented a community of young researchers, that interacted lively during talks, poster sessions (that featured a particularly positive atmosphere), discussion sessions (Q&A) and also during breaks; it allowed participants to interact with two scientific editors in relevant journals and to discuss critically the editorial landscape; all in all, we are sure IntCha24 allowed people to meet and know each other, to discuss new results and that it especially fostered new collaborations and strengthened the community as a whole. The focus of the conference on young researchers, the relaxed but scientifically intense poster sessions, and the general atmosphere have been cited, when asked for feedback, to be important factors of the event and pushed participants to declare themselves extremely satisfied and willing to participate again in similar further events. Thanks to the interdisciplinary nature of the conference, most participants declared to have gained new interests, specifically to more "fringe" topics in the community, such as information in biology and micro/nanofluidics.

Chemotaxis – from basic physics to biology
Workshop
Scientific coordinators: R. Insall, J. Simmchen

Impressions ...

... from the organisers: It was a very great success, in large part due to the MPI's facilities and expertise in planning, and we were delighted to see a number of your members attending the meeting, in different combinations for different talks, and joining in and contributing with vigour. Lots of new alliances and ideas were generated. Promoting truly cross-disciplinary work is challenging, but this meeting succeeded, with a satisfying level of engagement across disciplines from biology, engineering, chemistry, and mathematics. We both look forward to seeing your institute again, perhaps as attendees at a future meeting inspired by this one.

... from a participant: The biggest strength of this conference was its cross disciplinary scope. By bringing together perspectives from across a range of subjects and focussing them on one idea led to rich discussions.

... from an invited speaker: This in-house meeting was a fantastic experience, allowing me to interact with renowned scientists and young faculty fellows. It provided a wonderful platform to share ideas, discuss research, and foster international collaboration.

For a brilliant and inspiring opening, which set the creative and open spirit and conducted us throughout the entire meeting, Prof. Judith Armitage, emeritus at Oxford University and one of the pioneers in bacterial chemotaxis, gave an excellent historical abstract of the development of chemotaxis research in microbiology, spiced with her own experience and philosophical views on science - a true inspiration for all attendees.

Further highlights included:

- 16 invited speakers that joined us from all over the world to share their insights into a fascinating world of microagents migrating towards and away from food, danger or social interactions, all mediated through chemicals.
- Brilliant contributed talks that opened our eyes about all the exciting research that is going on around the globe - from Chile to China!
- Engaging poster discussions with early career researchers.
- Outreach talk - Dr. Christina Roggatz - 60 attendees including a class of pupils from Meissen, learning about the effects of pH on ocean chemistry and the way it changes animal behaviour and survival. Lively discussions and refreshments afterwards.
- Poster awards were funded by the RSC and awarded to Pieter de Visser and Barbara Borges Fernandes.
- The excursion on Wednesday was clearly a highlight: sunset hike with conference dinner at Pfaffenstein - we discussed new scientific ideas and exchanged about best practice in the lab, and therefore we have to disagree with Nature Physics! (Nat. Phys. 20, 677 (2024) - hikes are a great way to bring scientists together and talk!)

Disciplines involved ranged from biologists presenting stunning examples of the miracles nature has developed over the course of evolution, to physicists and mathematicians coming up with models to extract the basic information essential for understanding, engineers, chemists and interdisciplinary scientists trying to engineer artificial analogies.

Looking towards the future, we collectively identified challenges for the field:

- unify nomenclature
- continue to adapt methods across different disciplines
- translate findings across different research areas
- enhance communication to increase and improve the research perspectives
- formulate a hypothesis how chemotaxis evolved

To conclude, we very much enjoyed the coordination of this fruitful meeting, which reflected extremely well on the Max Planck society and its organisational framework. We will dedicate thoughts on how to continue the collaboration and keep the spirit of the meeting.

Flat bands and high-order Van Hove singularities
Seminar and Binodal Workshop
Scientific coordinators: C. Chamon, L. Classen, J. Betouras

The event FB-VHS 2024 was divided into a workshop week during May 27 – 31, 2024 and a following seminar week June 3 - 7, 2024. The first week was held in a novel format with participants meeting in two nodes in Daejeon, Korea, and in Dresden, Germany. Talks and question sessions were broadcasted life from each node. The workshop and seminar brought together scientists from experiment and theory working on the engineering, description, and consequences of flattened electronic bands, which can range from high-order Van Hove points to completely flat bands with or without topological character. In doing so, the aim of the workshop was to advance the field of quantum design of materials.

The workshop allowed the participants to approach the common theme of band flatting from different viewpoints. On the one hand, this means studying realisations in different material platforms such as correlated electron systems, designer heterostructures, or magnetic materials. On the other hand, this

involves utilising different methodologies from material synthesis and experimental techniques, over ab initio predictions and modelling, to topological analyses and many-body methods.

Over 70 participants from 12 countries attended the meeting from the Dresden node, with many more from the Daejeon node. The program included 50 invited talks, as well as two poster sessions, and ample time for discussion and collaboration. The focus of the first week was on presenting new results, while the second week emphasised collaborative aspects. During the workshop, several exciting results were presented on, e.g., quantum geometric effects by Youichi Yanase and Raquel Queiroz, on fractional quantum anomalous Hall states by Xiadong Xu, Nicolas Regnault, and Andrei Bernevig, on latest developments in twisted graphene structures by Eva Andrei, Shahal Ilani, and Siddharth Parameswaran, as well as non-twisted graphene systems by Andrei Chubukov and Thomas Weitz, on electronic mechanisms for superconductivity by Francesco Guinea and Jörg Schmalian, and on tuning correlated states around Van Hove singularities in kagome metals and strontium ruthenate by Haim Beidenkopf and Andrew Mackenzie. Many more high-level talks on relevant topics were given both by established experts and junior researchers in their field. All early-career researchers were invited to present a poster, and the poster sessions were well attended with lively discussions.

Overall, the intense exchange between participants from different sub-fields, both locally and between nodes, created a stimulating atmosphere.

The talks, discussions, and posters at FB-VHS 2024 demonstrated the rapid development in the field of correlated electrons in flat or flattened bands with promising prospects due to evolving experimental tuning techniques and theoretical methods. As a result, the workshop enabled advances in the direction of deliberate control over Van Hove singularities and band flattening in correlated electron systems, and the stabilization of novel ground states.

We would like to thank the wonderful team of the Max Planck Institute for the Physics of Complex Systems, as well as the IBS Center for Theoretical Physics of Complex Systems, for their excellent assistance and technical support.

Geometry and non-adiabatic responses in non-equilibrium systems
Workshop
Scientific coordinators: P. W. Claeys, N. Goldman, M. Kolodrubetz

The quantum geometry appears in various contexts in many-body quantum systems out of equilibrium, both as an object of fundamental importance and as a practical tool. Recent theoretical and experimental developments (including in quantum simulation, flat band physics, and quantum control) have spurred research on this geometry in various new directions, where different communities however use similar notions in different contexts and with a different toolbox. The international workshop on Geometry and non-adiabatic responses in non-equilibrium systems aimed at bringing together communities working on different aspects of quantum geometry and many-body quantum dynamics, with the goal of fostering collaborations and bringing on new research directions. This workshop was held in-person during the week of 17-21 June 2024. The format included 26 talks, comprised of 18 invited talks and 8 contributed talks, as well as two introductory lectures by Dries Sels (New York University) and Tomoki Ozawa (AIMR, Tohoku University). These lectures were aimed at introducing the general themes of the workshop to the different communities as well as the junior participants. Both speakers did so successfully and the inclusion of these introductions was positively commented on by a large part of the audience. The workshop also included two poster sessions totalling over 50 poster contributions, which were well attended and covered a wide range of topics.

The talks can be grouped together in different interconnected topics:

- Notions of quantum geometry beyond standard settings (Robert-Jan Slager, Jan Behrends, Clara Wanjura, André Eckardt)
- Geometry in flat bands and quantum Hall physics (Bruno Mera, Jie Wang, Armin Rahmani, Grazia Salerno, Johannes Hofmann)
- Quantum simulation (Hannah Price, Gil Refael, Qingyun Cao)
- Quantum geometry and superconductivity (Eugene Demler, Bogdan A. Bernevig)
- Quantum geometry and quantum chaos (Anatoli Polkovnikov)
- Quantum control and counterdiabatic driving (Dries Sels, Adolfo Del Campo, Paul Schindler)
- Quantum geometry and driven quantum systems (Netanel Lindner, Iliya Esin, Takahiro Morimoto, Kater Murch)

- Quantum sensing (Fengnian Xia)

The workshop brough together leading experts from across the globe, both experimental and theoretical, and also included a large number of junior participants. We were impressed by the high quality and diversity of the contributions, which led to stimulating discussions throughout and addressed the topics we set out to cover, such that we believe the goal of the workshop was successfully achieved.

Non-equilibrium Many-body Physics Beyond the Floquet Paradigm
Workshop
Scientific coordinators: R. Moessner, G. Refael, H. Zhao

The conference titled "Non-equilibrium Many-body Physics Beyond the Floquet Paradigm" was dedicated to exploring the dynamics of quantum systems. These encompassed a wide range including electronic, atomic, synthetic systems, and quantum computing machines. The primary focus was on elucidating the behaviors of many-body quantum systems over time and under external drives.

The workshop featured a diverse array of speakers, both established leaders and emerging researchers in the field:

- Norman Yao (Harvard University)
- Soonwon Choi (MIT, remotely)
- Dmitry Abanin (Princeton University)
- Hannes Pichler (University of Innsbruck)
- Inti Sodemann (Leipzig University)

In addition to these prominent figures, the conference attracted numerous students, postdoctoral researchers, and junior faculty members. Many of these participants contributed through short talks and presentations during two dedicated poster sessions.

Recent years have witnessed significant advancements in the field of quantum dynamics, introducing novel concepts such as time crystals, multiply driven Floquet systems, and prethermalization mechanisms. The workshop served as a platform for presenting cutting-edge ideas and methodologies:

- Soonwon Choi and Daniel Mark introduced the concept of deep thermalization in atomic free evolving ensembles.
- Hannes Pichler proposed a new paradigm for quantum computing utilizing Rydberg atoms.
- Arnab Das presented new findings on unexplained steady states in periodically driven magnetic systems.
- Yang Peng introduced a novel local signature for identifying Floquet topological phases.

The conference underscored the evolving landscape of out-of-equilibrium quantum systems. As the field progresses towards achieving long-term control of coherent quantum devices, the concepts and results unveiled at the "Beyond Floquet" conference are poised to shape future research directions.

In conclusion, the workshop not only highlighted the latest achievements but also fostered discussions that are crucial for advancing our understanding and capabilities in non-equilibrium many-body physics.

Chemical Coding at the Atomic Scale: Designing Hybrid and Quantum Nanostructures for Applications in Optical Biosensing, Light Harvesting, Chiral Catalysis, and More
Workshop
Scientific coordinators: S. Erwin, A. Eychmüller, A. Govorov

Main Focus of Our Event. The workshop centered on the cutting-edge field of chemical coding at the atomic scale, covering a wide range of topics in nanomaterials science and technology. Key themes included:

- Nanoparticle synthesis, assembly, and applications: From colloidal quantum dots and perovskite nanocrystals to plasmonic nanostructures
- Biosensing and bioanalytics: Utilization of nanoparticles for advanced sensing and testing systems
- Optical and quantum properties: Exploration of excitonic effects, energy transfer, and quantum phenomena in nanostructures

- Chiral nanostructures: Synthesis, characterization, and applications of chiral nanomaterials
- Energy conversion and catalysis: Nanostructure-based systems for photocatalysis, electrocatalysis, and solar energy conversion
- Theoretical aspects: Electromagnetic theory and modeling of nanostructures
- Emerging applications: Quantum sensing, optoelectronics, and metamaterials

The program featured a mix of fundamental research and applied science, fostering discussions on the design, synthesis, characterization, and application of nanomaterials across various fields.

Most Important Participants. The workshop brought together 60 participants from 10 countries, representing a diverse range of expertise in nanomaterials and chemical coding. Notable attendees included:

- Dr. Alexander Efros (Naval Research Laboratory, USA), renowned for his work on semiconductor nanocrystals
- Prof. Hilmi Volkan Demir (Nanyang Technological University, Singapore & Bilkent University, Turkey), expert in colloidal quantum wells and optoelectronics
- Prof. Maksym Kovalenko (ETH Zürich, Switzerland), leading researcher in perovskite quantum dots
- Prof. Jochen Feldmann (Ludwig-Maximilians-Universität München, Germany), known for his work on semiconductor nanocrystals and energy conversion
- Prof. David J. Norris (ETH Zürich, Switzerland), expert in the synthesis and optical properties of nanocrystals
- Prof. Daniel Vanmaekelbergh (University of Utrecht, the Netherlands), specialist in the characterization and topology of 2D nanostructures
- Prof. Itamar Willner (The Hebrew University of Jerusalem, Israel), pioneer in nanozymes and DNA-protocell condensates

The diverse participation facilitated rich discussions and collaborations across various subfields of nanomaterial science and engineering.

Presentation of Scientific Newcomers. Early-career researchers and established scientists alike had opportunities to present their work and engage in scientific discourse:

- Two dedicated poster sessions (Tuesday and Thursday evenings) showcasing a wide range of novel research in nanostructure design, synthesis, and applications
- Numerous oral presentations throughout the week, allowing for in-depth discussions of cutting-edge research
- Ample time allocated for discussions after each session, fostering collaborative dialogue and idea exchange
- Informal networking opportunities during coffee breaks, meals, and social events, enabling newcomers to connect with established researchers

Scientific Results in the Broader Sense. The workshop yielded several significant outcomes:

- Identification of key research directions in nanocrystal synthesis, assembly, and applications
- Cross-disciplinary insights into the interplay between material properties and quantum phenomena in nanostructures
- New perspectives on chiral nanostructures and their potential in sensing and catalysis
- Discussions on standardizing characterization methods for optical and quantum properties of engineered nanomaterials
- Exploration of machine learning approaches for designing atomic-scale material functionalities

Overall, the workshop fostered a vibrant exchange of ideas, pushing the boundaries of our understanding in chemical coding at the atomic scale and setting the stage for future breakthroughs in nanomaterial applications across multiple technological domains.

Localization: Emergent Platforms and Novel Trends
Workshop
Scientific coordinators: F. Evers, I. A. Gruzberg, A. Mirlin

The subject of the Workshop was Anderson localization and many-body localization, with a particular focus on emergent experimental platforms and on novel directions in the field. The field of localization was understood rather broadly, so that adjacent research areas have also been represented. In some of these areas the understanding of relations to localization physics is currently emerging and is a subject of active investigations. This included, in particular, the areas of quantum dynamics in NISQ devices, phase transitions induced by quantum measurements, strongly correlated systems (spin liquids), and advanced computational approaches to complex systems (such as methods based on tensor networks).

The Workshop involved participation of both theorists and experimentalists. While most of the presentations were theoretical, there was also a considerable number of experimental talks that covered modern experimental platforms that are most relevant to current developments in the field, including cold atoms (also under periodic driving), superconducting qubit arrays, photonic structures, disordered superconducting films, and disordered semiconductors.

There was a large interest in the Workshop, so that, in view of the upper limit, we were not able to admit all applicants who would otherwise fully qualify. The number of participants of the Workshop was 105, representing 20 countries. The program included 31 invited talks, 16 contributed talks, and 46 posters. Most of the invited talks were given by leading experts in their respective fields. At the same time, several invited talks, many contributed talks, and most of the posters were presented by young scientists. This gave an outstanding opportunity for young researchers to present their results to an expert audience and to discuss them with leading people in the field.

In our view, and according to feedback from many participants, the Workshop was very successful. After each talk, there were many questions and intense discussions, that often had to continue during coffee breaks, lunches, and dinners. There were many interconnections between the talks, which also promoted stimulating discussions. During the poster sessions, the activity of participants was also remarkably high, with vivid discussions of poster contributions until late in the evening (10 pm). The very fruitful exchange of ideas during the Workshop stimulated many collaborations between the participants and gave a boost to the research field.

We would like to thank the Institute staff, and in particular Claudia Domaschke, for outstanding organizational support. We are also very thankful to Ronny Börner for support on the IT side. Furthermore, we express our sincere gratitude to the Ph.D. students — Wouter Buijsman, Giovanni Cemin, Michael Sonner and James Walkling — who provided the IT assistance during the sessions. It is worth emphasizing that this was not always an easy job for the students, as they are not IT professionals.

Matter to Life Fall Days
Symposium
Scientific coordinators: J. Heidelberger, D. Madhavan, F. Jülicher

The Max Planck School Matter to Life holds biannual conferences, which are primarily for the Fellows (PIs/ Professors) and students of the school. Each edition of the conference is hosted by one of its partner institutes, and this fall mpi**pks**, under the guidance of Frank Jülicher, had the pleasure of hosting the event. The topic of the conference could be described under the broad umbrella of Matter to Life, which is an interdisciplinary approach to study how, when and why matter transitions to life, and the physical, chemical and biological principles of this.

Matter to Life fellows from Dresden, Anthony Hyman & Stephan Grill (MPI-CBG) and Stefan Diez (TU Dresden), were joined by those from other parts of Germany. This included Tobias Erb & Victor Sourjik (MPI-Terrestrial Microbiology, Marburg), Andrea Mussachio (MPI-Molecular Physiology, Dortmund), Andrij Pich (DWI-Leibniz Institute, Aachen), and Tanja Weil (MPI-Polymer Research, Mainz). Their talks on their current research along with those from senior PhD candidates of the school, covered a wide array of topics; biomolecular condensates, mechanics of nuclear periphery, motility in bacteria or diatoms, colloidal systems and their applications, to name a few.

The talks were supplemented by a workshop conducted by members of Thorsten Moos's group (Heidelberg University) on ethics of synthetic organoids. Students took center stage and played members of an ethics committee to decide the fate of a hypothetical project that pushed the boundaries of our current ethical considerations. The poster presentation session and the lab visits to MPI-CBG ensured the program was

interactive and dynamic for early-stage students and researchers. The program concluded with a keynote speech by Miki Ebisuya (TU Dresden), who presented her fascinating work on biological clocks, and the development of a Stem cell zoo in order to better answer her research questions.

The attendees were Faculty and students from diverse backgrounds of Physics, Chemistry and Biology, and this guaranteed a truly interdisciplinary discussion, knowledge exchange, and hopefully fruitful collaborations in the field of Matter to Life.

Quantum Meets Classical
Workshop
Scientific coordinators: A. Chandran, S. Gopalakrishnan, C. Laumann, V. Oganesyan

The goal of this workshop was to bring together scientists working at the interface where quantum systems meet the classical world. This is a broad area but several scientific clusters naturally emerged in the course of the workshop, reflecting the state of the field. Broadly, these themes included

- simulating quantum and classical statistical mechanical phases and phase transitions on current quantum processors;
- the emergence of both normal and anomalous hydrodynamic descriptions from quantum dynamics (primarily in 1D);
- methods to generate useful entanglement from hydrodynamic processes;
- the complex relationships between semi-classical dynamics, scars, chaos and entanglement generation;
- the physics and mathematics of random unitary and monitored circuits;
- classical computational techniques exploiting entanglement and symmetry to simulate quantum phases and dynamics;
- Anderson localization in high dimensions and its relationships with coding.

The workshop kicked off on Monday evening with a colloquium and welcome dinner, which set the stage for the primary series of 24 talks spread over the next four days. Talks were allocated longer format 45 minute slots, which enabled speakers to provide pedagogical introductions with ample space for questions, of which there were many. Some 26 contributed posters anchored the evening poster sessions on Tuesday and Thursday, which were well attended and busy with discussion. These were an especially useful opportunity for junior participants to present their work and interact with other participants. Finally, the Wednesday afternoon hike in the Sächsische Schweiz was a perfect, anomalously sunny and beautiful, break and setting for longer informal discussions.

3.4 Collaboration with Experimental Groups

- *Bacterial motion* with W. C. K. Poon, University Edingburgh (UK)
- *Phoretic colloids* with D. J. Kraft, Universiteit Leiden (Netherlands)
- *Microfluidics, sperm motility* with H. A. Stone, Princeton University (USA)
- *Active transport in porous media* with S. S. Datta, Caltech (USA)
- *C. elegans gonad mechanics* with S. Grill, MPI-CBG (Germany)
- *Morphogenesis in Volvocaceae* with S. Höhn, Cambridge (UK)
- *Mechanical instabilities in cysts* with A. Honigmann, TU Dresden (Germany)
- *Mechanics of cysts* with A. Janshoff, University Göttingen (Germany)
- *Tissue folding in the developing zebrafish brain* with M. Smutny, University of Warwick (UK)
- *Morphogenesis of the Drosophila hindgut* with S. Shvartsman, University of Princeton/Flatiron Institute (USA)
- *Drosophila gastrulation mechanics* with P. Tomancak, MPI-CBG (Germany)
- *Mechanics of apical bulkheads in the liver and liver morphogenesis* with M. Zerial, MPI-CBG (Germany)
- *Assembly of Rydberg molecules in optical tweezers* with S. Cornish, A. Guttridge, Durham University (UK)
- *High-precision spectroscopy of trilobite Rydberg molecules* with H. Ott, TU Kaiserslautern-Landau (Germany)
- *Non-adiabatic physics of low-n Rydberg molecules* with J. Hecker Denschlag, Ulm University (Germany)
- *Collective cell migration* with X. Trepat, Institute of Bioengineering of Catalonia, IBEC (Spain)
- *Self-organization in colonies of motile soil bacteria* with J. Shaevitz, Princeton University (USA)
- *Cell migration guidance* with R. Mayor, University College London (UK)
- *Collective behavior of active colloids* with J. Zhang, University of Science and Technology (China)
- *Bacterial biofilms* with J. Yan, Yale University (USA)
- *Collective migration and organization of neural crest cells* with E. Barriga, Cluster of Excellence Physics of Life, TU Dresden (Germany)
- *Embryo implantation as active wetting* with K. Cavanaugh, University of California (USA)
- *Pattern formation in actomyosin networks* with S. Grill, MPI-CBG (Germany)
- *Applications of prethermal states of matter induced by periodic pulsed drives in nitrogen-vacancy centers in diamond* with A. Ajoy, UC Berkeley (USA)
- *Topological photonics* with K. Leo, TU Dresden (Germany)
- *Emergence of strong correlations in the pseudogap phase of a Fermi-Hubbard quantum simulator* with I. Bloch, T. Hilker, T. Chalopin, LMU Munich, MPI for Quantum Optics (Germany)
- *Feshbach spectroscopy of the atrractive Hubbard model* with M. Zwierlein, Massachusetts Institute of Technology, Boston (USA)
- *Elastocaloric effect of SrCu2(BO3)2 under uniaxial pressure* with E. Gati, F. Liebrich, MPI for Chemical Physics of Solids (Germany)
- *Tissue scaling and growth control* with M. Gonzales-Gaitan, Universite de Geneve (Switzerland)
- *Active cellular processes* with P. Martin, Institut Curie, Paris (France)
- *Physics of biomolecular condensates* with T. Hyman, MPI-CBG Dresden (Germany)
- *Branching morphogenesis and organism scaling* with J. Rink, MPI-BPC Göttingen (Germany)
- *Material properties of condensates* with L. Jawerth, Leiden University (Netherlands)

3.5 Externally Funded Research and Relations to Industry

3.5.1 DFG Projects

- Gottfried Wilhelm Leibniz-Preis 2013, Prof. R. Moessner
- Gottfried Wilhelm Leibniz-Preis 2017, Prof. F. Jülicher
- Collaborative Research Center 1143 *Correlated magnetism: from frustration to topology*, Prof. R. Moessner

- Research Group FOR5522 *Quantum Thermalization, Localization, and Constrained Dynamics with Interacting Ultracold Atoms*, Prof. R. Moessner
- *Kontrolle von Ionisation durch die zeitliche Änderung der Pulsform des Lichts*, Prof. J.-M. Rost, Prof. Dr. U. Saalmann
- Exzellenzcluster *Physics of Life*, Prof. F. Jülicher
- Exzellenzcluster *Complexity and Topology in Quantum Matter*, Prof. R. Moessner

Individual Projects

- *Die Entstehung von phasengetrennten Transkriptionszentren und ihre Funktion in der Transkriptionsregulation*, Dr. J. Brugués
- *Prinzipien der räumlichen und zeitlichen Kontrolle der Initiation meiotischer Rekombination in Mäusen*, Dr. S. Rulands
- *Exzitonentransport und optische Eigenschaften von Quantenaggregaten*, Dr. A. Eisfeld
- *SuMaC: Supraleitung und magnetische Korrelationen*, Dr. A. Wietek
- *Die Faltung von Eithelewerbe als morphogenisches Werkzeug*, Dr. M. Popović
- *Die Quantenthemalisierung, Lokalisierung und eingeschränkte Dynamik mit wechselwirkenden ultrakalten Atomen*, Prof. R. Moessner
- *Heterostrukturen zur Erforschung altermagnetischer und supraleitender Spintronik*, Dr. L. Šmejkal

3.5.2 EU Funding

- EU - Horizont 2020 *Climate Advanced Forecasting of Sub-seasonal Extremes (CAFE)*, Prof. Dr. H. Kantz
- EU - ERC STG *The Spectrum of Fluctuations in Living Matter*, Dr. R. Alert
- EU - ERC STG *Understanding collective mechanisms of cell fate regulations using single-cell genomics*, Dr. S. Rulands
- EU - ERC STG *Nonequilibrium Many Body Control of Quantum Simulators*, Dr. M. Bukov
- EU - ERC STG *Magnetic counterparts of unconventional superconductors for spin-conserved and non-dissipative electronics*, Dr. L. Šmejkal
- EU - MSCA *Off-resonant parametric control over THz collective modes in correlated materials: Complex driving protocols, non-equilibrium correlated states and applications*, Dr. E. Kiselev
- EU - MSCA *General Eigenstate Thermaliation in Quantum Circuits*, Dr. F. Fritzsch

3.5.3 Additional External Funding

- VW *The spark of life: initiation of transcription in embryos, and recapitulating such in synthetic nuclei*, Dr. J. Brugués
- VW *Interplay of Proteins and Nucleic Acid Polymers in Compartment Formation*, Prof. Dr. F. Jülicher
- SAB *Treatment decision based on organoids in gastric cancer*, Prof. Dr. F. Jülicher
- BMBF *CompLS - Runde 1 - Einzelprojekt: SPlaT-DM- Computersimulationsplattform für Topologiegesteuerte Morphogenese*, Dr. C. Modes
- BMBF *Skalierbare Synchronisation in Netzwerken elektronischer Taktgeber bei zeitverzögerten Kopplung und flacher Hierarchie - PLL Synchronisation (Verbundprojekt) Teilvorhaben: Modellierung, Bootstrategie, Kontrolle der Dynamik und Koordination*, Dr. L. Wetzel

3.5.4 Scholarships

- Linge Li; China Scholarship Council
- Royota Takaki; Japan Society for the Promotion Science
- Akhie Varma; AvH
- Pallabi Das; AvH

3.5.5 External Cofunding of Workshops and Seminars

2022

- Focus Workshop *Physics and Collective Dynamics of Future Mobility*
  (93 % of budget)
- Focus Workshop *Topological Materials: From Weak to Strong Correlations*
  (38 % of budget)
- Workshop *New Trends in Nonequilibrium Many-Body Systems: Methods and Concepts*
  (15 % of budget)
- Workshop *Quantum Transport with ultracold atoms*
  (15 % of budget)
- Workshop *Topology and non-equilibrium dynamics in engineered quantum systems*
  (69 % of budget)

2023

- School *Spring School on Modern Topics in Condensed Matter*
  (84 % of budget)
- Workshop *Quantum Materials in the Quantum Information Era*
  (20 % of budget)
- Seminar and Workshop *Non-autonomous Dynamics in Complex Systems: Theory and Applications to Critical Transitions*
  (18 % of budget)
- Focus Workshop *Quantum thermalization, localization, and constrained dynamics with interacting ultracold atoms*
  (100 % of budget)

2024

- Workshop *Quantum Interactive Dynamics*
  (37 % of budget)
- Workshop *Interdisciplinary challenges in non-equilibrium physics: from soft to active, biological and complex matter*
  (7 % of budget)
- Workshop *Chemotaxis – from Basic Physics to Biology*
  (28 % of budget)
- Seminar and Binodal Workshop *Flat bands and high-order Van Hove singularities*
  (6 % of budget)
- Workshop *Chemical Coding at the Atomic Scale: Designing Hybrid and Quantum Nanostructures for Applications in Optical Biosensing, Light Harvesting, Chiral Catalysis, and More*
  (38 % of budget)
- Focus Workshop *Localization and Constrained Dynamics in Quantum Many-Body Systems*
  (100 % of budget)

3.5.6 Patents and Licenses

- *J. Götte, R. Cameron, S. Barnett*
  International patent **PCT/EP2016/076742**
  Chiral rotational spectrometer, since 11/2015
- *A. Pollakis, L. Wetzel, D. J. Jörg, W. Rave, F. Jülicher, G. Fettweis*
  European patent **EP 2 957 982**
  Self-synchronizable network, since 08/2017

3.6 Teaching and Education

3.6.1 Lectures at Universities

Wintersemester 2021/22

- *Nonlinear Dynamics* Prof. Dr. Holger Kantz, TU Dresden
- *Theory of energy transfer and optical response in quantum assemblies* Dr. Alexander Eisfeld, TU Dresden
- *Theory of open quantum systems for molecules* Dr. Alexander Eisfeld, TU Dresden

Sommersemester 2022

- *Nonlinear Dynamics* Prof. Dr. Holger Kantz, TU Dresden
- *Hypothesis Program in Quantitative Biology and Ecology* Dr. Ricard Alert, ICTP-SAIFR, Sao Paulo

Wintersemester 2022/2023

- *Stochastic Processes* Prof. Dr. Holger Kantz, TU Dresden
- *Introduction to Unitary Circuit Dynamics* Dr. Pieter Claeys, Stony Brook University
- *Rydberg physics of atoms, molecules, and ultracold gases* Dr. Matt Eiles, TU Dresden

Sommersemester 2023

- *Nonlinear Dynamics* Prof. Dr. Holger Kantz, TU Dresden
- *Advanced Biological Physics* Dr. Pierre Haas, Dr. Ricard Alert, TU Dresden
- *Quantum Mechanics II* Dr. Alexander Eisfeld, Uni Potsdam
- *The Physics of Photosynthesis* Dr. Alexander Eisfeld, Uni Potsdam

Wintersemester 2023/2024

- *Atmospheric Physics* Prof. Dr. Holger Kantz, TU Dresden
- *Many-Body Quantum Dynamics* Prof. Dr. Roderich Moessner, Dr. Marin Bukov, Dr. Pieter Claeys, TU Dresden
- *Pattern Formation in Biology* Dr. Pierre Haas, Dr. Ricard Alert, Dr. Marko Popović, TU Dresden
- *Geometry and Topology in Quantum Physics* Prof. Dr. Jan Budich, TU Dresden
- *Active Matter Hydrodynamics* Prof. Dr. Frank Jülicher, Prof. Dr. Stephan Grill, Dr. Marko Popović, TU Dresden

Sommersemester 2024

- *Advanced Biological Physics* Dr. Christina Kurzthaler, Dr. Pierre Haas, Dr. Ricard Alert, TU Dresden
- *Quantum Mechanics II* Dr. Alexander Eisfeld, Uni Potsdam
- *The Physics of Photosynthesis* Dr. Alexander Eisfeld, Uni Potsdam
- *Rydberg physics of atoms, molecules, and ultracold gases* Dr. Matt Eiles, TU Dresden
- *Quantentheorie II* Prof. Dr. Jan Budich, TU Dresden

Wintersemester 2024/2025

- *Stochastic Processes* Prof. Dr. Holger Kantz, TU Dresden
- *Many-Body Quantum Dynamics* Prof. Roderich Moessner, Dr. Marin Bukov, Dr. Pieter Claeys, TU Dresden
- *Pattern Formation in Biology* Dr. Pierre Haas, Dr. Marko Popović, TU Dresden
- *Computational Tools for Quantum Many-Body Physics* Prof. Dr. Jan Budich, TU Dresden
- *Active Matter Hydrodynamics* Prof. Dr. Frank Jülicher, Prof. Dr. Stephan Grill, Dr. Marko Popović, TU Dresden

3.6.2 Professional Skills Training

Talk series on professional skills topics

- *From Quantum Mechanics to Neural Networks: My Transition from Academic Physics to AI in the Tech Industry*
  Heiko Burau, elevait GmbH Dresden(November 2023)
- *Data Careers in the 2020s*
  Dr. Chris Armbruster, Data Science Retreat Berlin (November 2022)
- *From a PhD to a Team Master at TraceTronic GmbH Dresden*
  Paula Ostmann, TraceTronic GmbH Dresden (July 2022)
- *Powerpoint and Petrol - Working in Automotive Development, Engineering as a Physicist*
  Maximilian Buchholz, University of California, Berkeley (October 2021)

3.6.3 Degrees

Dissertations

- Bauermann, J.: *Organization of chemical reactions by phase separation* Dresden, 2022
- Colmenarez, L.: *Fast, slow and super slow quantum thermalization* Dresden, 2022
- Eidi, M. R.: *Basis sets for light-matter interaction: From static coherent states to moving Gaussians* Dresden, 2022
- Lopez, A. A.: *Structuring microscopic dynamics with macroscopic feedback* Dresden, 2022
- Miranda, M.: *The Dynamics of Active Filaments* Dresden, 2022
- Mukherjee, A.: *Physics of Oocyte Growth and Selection: A Mesoscopic Perspective* Dresden, 2022
- Olmeda, F.: *Non Equilibrium Physics of Single-Cell Genomics* Dresden, 2022
- Schaefer, R.: *Magnetic frustration in three dimensions* Dresden, 2022
- Szabo, A. L.: *From electronic correlations to higher-order topology in nodal Fermi liquids* Dresden, 2022
- Verdel Aranda, R.: *Nonequilibrium dynamics in lattice gauge theories: Disorder-free Localization and string breaking* Dresden, 2022
- Azizi, S.: *Three aspects of photoionization in ultrashort pulses* Dresden, 2023
- Bartolucci, G.: *Control of condensate shape and composition via chemical reaction networks* Dresden, 2023
- Corticelli, A.: *Symmery and Magnon Band Topology: Constraint and Enrichment* Dresden, 2023
- Gemsheim, S.: *The emergence of time with interactions in quantum and classical mechanics* Dresden, 2023
- Hu, X.: *Estimating prediction skill of El Nino Southern Oscillation (ENSO) and its teleconnection on precipitation anomalies* Dresden, 2023
- Janssen, J.: *Coarsening Kinetics of Chemically-Active Emulsions* Dresden, 2023
- Johansen, C.: *Field theory of interacting polaritions under drive and dissipation* Dresden, 2023
- Laha, S.: *Chemical reactions controlled through compartmentalization: Applications to bottom-up design of synthetic life* Dresden, 2023
- Mantilla Serrano, S. F.: *Hard-core bosons in phase diagrams of 2D Lattice Gauge Theories and bosonization of Dirac fermions* Dresden, 2023
- McRoberts, A. J.: *Anomalous spin dynamics in low-dimension: Superdiffusion, Subdiffusion and Solutions* Dresden, 2023
- Meigel, F.: *Multi-scale fluctuations in non-equilibrium systems* Dresden, 2023
- Placke, B.: *Exotic Ground States and Dynamics in Constrained Systems* Dresden, 2023
- Rao, P.: *Spin-anyon duality and Z2 topological* Dresden, 2023
- Rouges, E.: *European heatwaves: intraseasonal drivers and prediction* Dresden, 2023
- Wastiaux, A.: *Study of topological and transport properties of spin-orbit coupled Josephson junctions* Dresden, 2023
- Bonifacio, M.: *Exploiting the cavity time scale to engineer interactions in quantum gas* Dresden, 2024

- Hahn, D.: *Non-equilibrium dynamics and information spreading in many-body quantum systems* Dresden, 2024
- Hanauer, Ch.: *Pattern Formation and Branching in Morphogen-controlled Interface Growth* Dresden, 2024
- Jha, M. Ch.: *Topological phases on non-periodic lattices* Dresden, 2024
- Kassel, J. A.: *Nonlinear Long-Range Correlated Stochastic Models of Temperature Time Series: Inference and Prediction* Dresden, 2024
- Mohammadzadehhashtroud, A.: *Collective Processes in Cellular Reprogramming* Dresden, 2024
- Neipel, J.: *Geometric Control of Active Flows* Dresden, 2024
- Rabe, St. B.: *Diabatization via Gaussian Process Regression* Dresden, 2024
- Sarangi, S.: *Topological phases in self-similar systems* Dresden, 2024
- Streissnig, C.: *Stochastic Aspects of the Second Law of Thermodynamics* Dresden, 2024
- Stefanidis, N.: *Symmetry breaking and fractionalization in Landau levels & flat topological insulator* Dresden, 2024

Master Theses

- Shinde, R.: *Information Processing and Energetics in a Multiscale Demonic System.* Dresden, 2022
- Laxhuber, K.: *Stochastic Thermodynamics of Active Droplets.* Göttingen, 2023
- Maximova, E.: *Temporal correlations in active nematic turbulence.* Dresden, 2023
- Lee, S.: *Tissue Folding as a Morphogenetic Mechanism.* Göettingen, 2023
- Manna, A.: *Electrohydraulicss of Epithelium.* Göttingen, 2023
- Mascarenhas, T.: *Stochastic Thermodynamics of Cellular Information Processing.* Göttingen, 2023
- Geerds, B. C.: *Spatio-Temporal Control of Topological Defects in Active Matter.* Dresden, 2024

Bachelor Theses

- Jans, A. N.: *Gangdaten von Pendeluhren als Indikatoren Physikalischer Einwirkungen* Dresden, 2022
- Loth, J. P.: *Extremwertstatistik für Niederschlagsmengen* Dresden, 2024

3.6.4 Appointments and Awards

Appointments

- Dr. J. O. Benton accepted the offer for a lectureship at the *Queen Mary University, London, United Kingdom*.
- Dr. S. Bo accepted the offer for a lectureship at the *King's College London, United Kingdom*.
- Prof. J. Brugés accepted the offer for a professorship at the *Technische Universität Dresden, Germany*.
- Dr. S. Choubey accepted the offer for a readership at the *Institute of Mathematical Sciences, Chennai, India*.
- Prof. C. Datt accepted the offer for an assistant professorship at *Keio University, Japan*.
- Prof. Ch. Duclut accepted the offer for an associate professorship at *Sorbonne Université Paris, France*.
- Prof. A. Eisfeld has a deputy professorship at *University of Potsdam, Germany*.
- Prof. T. Han Tan accepted the offer for an assistant professorship at the *University of California, San Diego, United States*.
- Prof. S. Hegde accepted the offer for an assistant professorship at the *Indian Institute of Science Education and Research Thiruvananthapuram, India*.
- Prof. C. Hooley accepted the offer for a professorship at *Coventry University, United Kingdom*.
- Prof. V. Ivády accepted the offer for an assistant professorship at *Eötvös Loránd University, Budapest, Hungary*.

- Prof. I. Khaymovich accepted the offer for an assistant professorship at the *Nordic Institute of Theoretical Physics, Stockholm, Sweden*.
- Prof. F. Piazza accepted the offer for a professorship at the *University of Augsburg, Germany*.
- Dr. P. Pietzonka accepted the offer for a lectureship at the *University of Edinburgh, United Kingdom*.
- Prof. I. Sodemann accepted the offer for a professorship at the *University of Leipzig, Germany*.
- Prof. S. Rulands accepted the offer for a professorship at the *Ludwig-Maximilians Unviersity, Munich, Germany*.
- Prof. T. Wasak accepted the offer for an assistant professorship at the *Nicolaus Copernicus University, Toruń, Poland*.
- Prof. S. Zhang accepted the offer for an assistant professorship at the *Okinawa Institute of Science and Technology, Japan*.
- Prof. H. Zhao accepted the offer for an assistant professorship at *Peking University, China*.

Awards

- Alert, R.: *Antalgenics Prize 2022, by the Spanish Society of Biophysics*.
- Alert, R.: *IUPAP Early Career Prize 2023*.
- Alert, R.: *ERC starting grant*.
- Alert, R.: *Finalist of Princesa de Girona Research Prize, by Fundacio Princesa de Girona*.
- Brugés, J.: *ERC consolidator grant*.
- Bukov, M.: *Outstanding Editorial Board Member, Nature Communications Physics 2022*.
- Bukov, M.: *ERC starting grant*.
- Bukov, M.: *John Atanasoff Award 2023*.
- Bukov, M.: *Fellow of the Young Academy of Europe, 2024*.
- Jülicher, F.: *Elected Member of the Deutsche Akademie der Naturforscher Leopoldina*.
- Jülicher, F.: *IUPAP Medal for the Physics of Life 2023*.
- Lenggenhager, P.: *SPS Thesis Award for Condensed Matter Physics*.
- Lenggenhager, P.: *ETH Silver Medal for outstanding PhD thesis*.
- Rulands, S.: *Funding for individualized cancer therapy from the Sächsische Wissenschaftsministerium*.
- Šmejkal, L.: *ERC starting grant*.
- Šmejkal, L.: *Walter Schottky Prize 2025, by the German Physical Society*.

3.7 Public Relations

3.7.1 Long Night of the Sciences

Over the last years, the institute has participated in the annual *Long Night of the Sciences*. Jointly with the Technische Universität Dresden and many other research institutes in Dresden, we opened our doors for the general public from 6pm to midnight. The members of our institute conveyed the importance and fascination of their research to a broad audience with various talks, shows, a science cinema, posters and a lot of different presentations of their work. The resonance was very good, with about 2000 visitors counted at each event.

Long Night of the Sciences © Sven Döring

3.7.2 Science in the Theater

The **mpipks**, the Technische Universität Dresden and the City of Dresden run a series of public lectures by leading scientists who explain their field of research to a lay audience. Since 2011 the three annual lectures have taken place in the "Kleines Haus" of Dresden's State Theater.

Figure 1: Science in the Theatre © Rene Gaens

3.7.3 mpipks School Contact Program

The **mpipks** offers high school classes the opportunity to catch a glimpse of the day-to-day life of a scientist. Every year, about nine classes visit us to attend a lecture by a junior member of the institute, who presents his field of research and answers questions about studying science, pursuing a PhD, etc.

In addition, the institute participates in the program *Junior Doctor* organized by the network *Dresden - Stadt der Wissenschaft*. The participating research institutes offer a variety of lectures for children, who are awarded a "Junior Doctor degree" when attending a stated number of talks.

Figure 2: Public lecture for Junior Doctors

3.7.4 30 years of the Max Planck Society in Saxony

MAX PLANCK INSTITUTE IN SACHSEN

30 JAHRE

30 years of the Max Planck Society in Saxony: Finisage on September 25, 2023 © Sven Döring

On September 4, 2023, Minister-President Michael Kretschmer and Max Planck President Patrick Cramer co-hosted a ceremonial event at the Kulturpalast in Dresden, commemorating the 30-year success story of the Max Planck Society in Leipzig and Dresden. Nobel Laureate Svante Pääbo from the Max Planck Institute for Evolutionary Anthropology in Leipzig gave a talk about his research on Neanderthals.

The foundational history of the Max Planck Society's research institutions in the eastern German states began on July 3, 1990. The first Institute in Saxony, the Max Planck Institute for Physics of Complex Systems in Dresden, started its work in the summer of 1993. Five more Institutes followed suit. Reflecting on this time, the then President of Max Planck Society, Hubert Markl, wrote in the late 1990s: "Creating such innovation across various scientific areas in the Max Planck Society was not only a unique challenge, but also an exciting experience."

At the same time, the Max Planck Society celebrated its 75th anniversary in 2023. This was an opportunity to celebrate excellent research 'Made in Saxony' and present it to the public. Research at the six Max Planck Institutes in Saxony was presented at numerous events, the schedule for which can be found at: https://www.mpi-cbg.de/30-years-max-planck-institutes-saxony

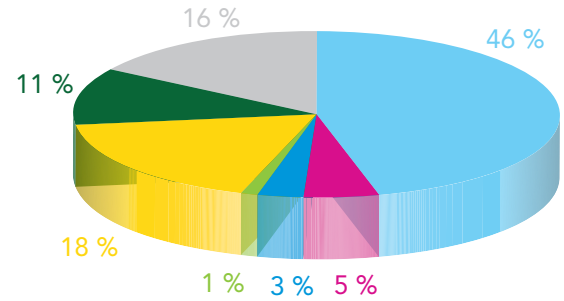
3.7.5 Scientific Workshop: 30 years MPI-PKS September 6 - 9, 2023

Figure 3: Scientific Workshop: 30 years MPI-PKS September 6 - 9, 2023 © Sven Döring

As the Max Planck Society celebrated being active in the state of Saxony for 30 years, the Max Planck Institute for the Physics of Complex Systems also turned 30. On this occasion, the institute organized an alumni workshop. Together, we wanted to find out and reflect upon the progress that has been achieved through the research of the institute's alumni over the years. Different generations of alumni had the opportunity to share their experiences among each other, as well as with current scientists in residence, through plenary and parallel talks and ample time for discussions. One talk session took place in the center of Dresden, open to the general public, as part of Saxony's Max Planck Society celebration.

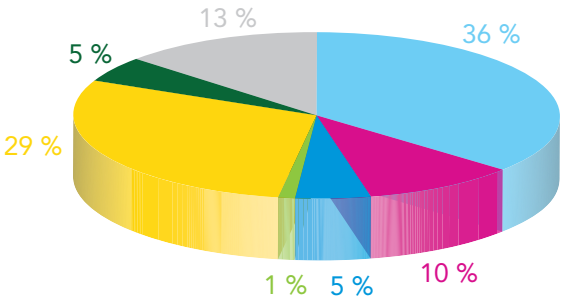
3.8 Budget of the Institute

Research Budget 2022



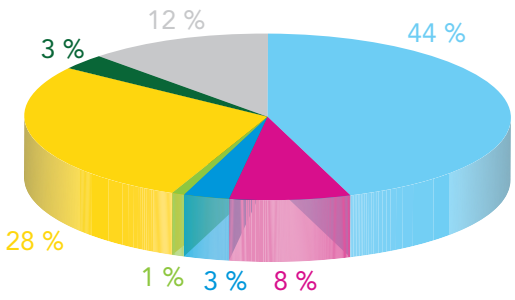
- Investment costs (IT/others)
- Workshops/Seminars (guest program)
- IT-costs
- Library costs
- Building management costs
- Building maintenance costs
- Other scientific costs

Research Budget 2023



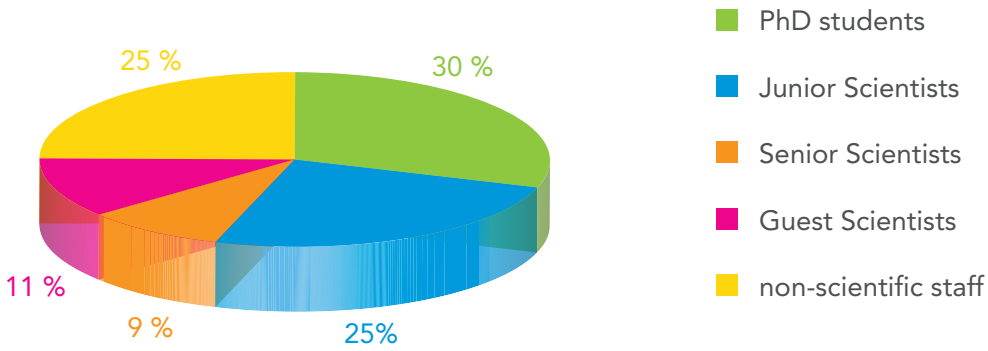
- Investment costs (IT/others)
- Workshops/Seminars (guest program)
- IT-costs
- Library costs
- Building management costs
- Building maintenance costs
- Other scientific costs

Research Budget 2024

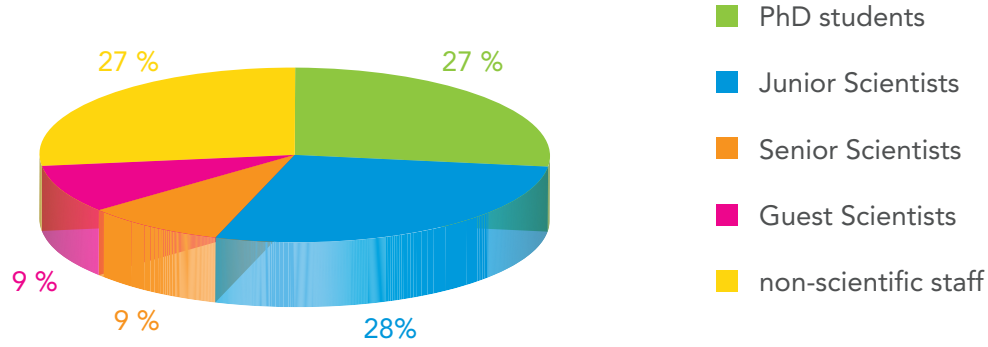


- Investment costs (IT/others)
- Workshops/Seminars (guest program)
- IT-costs
- Library costs
- Building management costs
- Building maintenance costs
- Other scientific costs

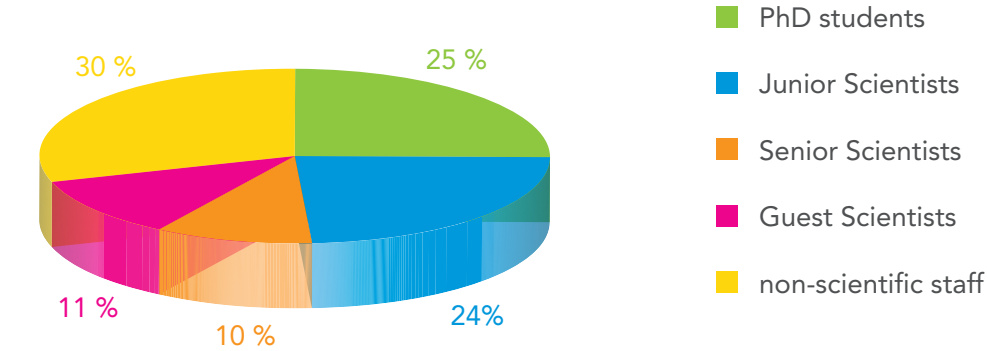
Personnel Budget 2022



Personnel Budget 2023



Personnel Budget 2024



3.9 Equipment and Premises

3.9.1 Computing Facilities

As a consequence of the Russian attack against Ukraine in 2022 the price for electric energy rose to an extremely high level, forcing us to save as much energy as possible. One of the consequences was that we now have all servers automatically switched off once they are not needed by any user's computing jobs. Another one was to reduce the number of jobs actually scheduled to our queuing system. This was a completely new situation both for the computer department and our users, since before the main goal was to equip the institute with as much computing power as possible. During the last months of 2022 and throughout 2023 we were able to save 20% of electric energy compared to the years before. Luckily the situation has improved, so that we do not have to put restrictions any more on the number of jobs our scientists are allowed to run.

Our seminar room

One of the main projects in 2022 was to equip our largest seminar room with technical devices suitable for hybrid formats of scientific seminars and workshops which became common due to the restrictions imposed by the Covid pandemic in 2020 - 2021. The key features of our equipment are ceiling microphones which allow people to be heard from everywhere within the seminar room, several cameras, a large display in the front and a software setup which permits to realize a very wide variety of configurations, including a setup for events located on two different sites with many participants on both sides.

Due to the relatively wide field of theoretical physics covered by our scientists there is a very broad spectrum of requirements that our IT facilities have to cope with. This implies in particular that compute nodes of very different size have to be available on site for numerical calculations. The complexity is luckily reduced by the fact that nowadays most scientific applications can be run on a Linux operating system, such that presently our computing facilities are homogeneous in the sense that both the hardware architecture (x86-64) and the operating system are the same throughout our cluster, including our workstations.

The close past has seen a slight increase in the requirements for graphics, partly due to activities in our Biological Physics department but also driven by the fact that visualization of results has become more important. At the same time the possibility to develop programs which make heavy use of GPUs was requested by our scientists. This is why we complemented our local cluster with several nodes with powerful GPUs during the last years. A new powerful cluster with fast GPU cards shared by the MPI for the Structure and Dynamics of Matter (Hamburg) and our institute was put in operation in 2022. This cluster was approved and subsidized by the BAR in 2021.

Since early 2019 we are hosting part of our cluster at the Lehmann Zentrum of the TU Dresden which is located just a few hundred metres away from our institute. This relatively new building has a perfect infrastructure for running large clusters, in particular it provides very efficient cooling. Due to the short distance we are able to integrate the computers there into our cluster in such a way that our users will not notice any difference compared to those located inside our own building.

As there is an ever growing requirement for more computing power by our scientists, our main server room had to be upgraded both with respect to power supply and cooling capacity. At the same time the usual server racks were to be replaced with racks with an heat exchanger in the rear door, providing more efficient cooling. This construction work was successfully finished late 2021. This gives us enough

capacity to run new air-cooled servers for the coming years, at the same time making the cooling much more efficient than it was before.

All of our offices are equipped with workstations in order to provide our scientists with a device that can run small applications and produce graphical output. For more elaborate calculations the institute hosts approximately 1000 servers with a total of approximately 92,000 CPU cores on site.

Our compute nodes have up to 192 CPU cores and a maximum of 6 Terabytes of main memory and a maximum of 28 Terabytes of local disk space. Several nodes with powerful GPUs are available for our scientists. We run 100, 10 and Gigabit Ethernet as a local area network interconnect. In order to maximize the computational throughput in our computing cluster, we run a network queuing system. Besides the unix cluster there are about 20 PC's in our institute, running a Windows operating system, mainly for office applications. We also offer about 120 laptops for our scientists in order to provide them with the possibility to continue their work while they are traveling or at home. Cloud services, VPN access, Wifi, including Eduroam and other services are also available for our scientists. For numerical and analytical calculations we offer various software packages. During the last few years we have noticed a tendency towards integrated software environments while fewer people are writing their own programs using programming languages like C, C++ or Fortran. In many cases a lot of the ongoing software development is done and driven by free software, e.g. in the Biological Physics department, though proprietary software also plays an important role at our institute.

We are connected to the Internet using a bandwidth of 1 GBit/s. Redundancy is achieved by automatic failover to a second line to our neighboring institute in case of problems with our primary Internet connection (and vice versa for their connection).

The computer department is run by five employees with their respective main tasks being Unix/Linux, Mac OS and cloud services, hardware and web, network and Windows, video conferencing. In addition to those five people we employ three trainees. Small to medium sized programming tasks are done by our staff and trainees. The development of large software applications, like a new database system for our visitors program or a refresh of our webpages, usually has to be implemented by external companies.

Future

As servers in the HPC area tend to show an ever growing power consumption with every new generation, there will be a tendency towards servers with direct cooling. This is presently already standard for the latest GPU generations which can no longer be cooled by air flow. While our facilities presently are not suitable for running servers with direct cooling, we could have such systems installed and running at either the MPCDF in Garching or at the Lehmannzentrum of the TU Dresden. The TU Dresden even uses heap pumps to bring the waste heat to a temperature suitable for feeding it into the district heating grid.

Artificial intelligence has been playing a role in theoretical physics for quite some time already. Presently it is unclear to which extent it will be necessary for our scientific research in the future and thus the amount of GPU based systems that will be required by our institute. For time being the cluster located at the MPCDF in Garching which we share with the MPI for the Structure and Dynamics of Matter is certainly sufficient. But there are hints that GPU based systems will become much more important in the not so far future.

Linux will continue to be the main operating system for our number crunchers in the near future, so far running on Intel Xeon and AMD EPYC based hardware. Presently it is still unclear if systems based on the ARM architecture will start to play a noticeable role in HPC clusters in the future. But there is a chance that they will come into play in the time frame of the next 2 - 3 years. Those CPUs may be less power consuming than the usual X86 architecture, which will make this technology quite interesting for us. Operating systems different from Linux, like AIX might only come into play if particularly fast hardware is required by our scientists that is not supported by Linux.

History

The following table shows the development of the computer resources on site at our institute in Dresden over time. The numbers do not include our parallel cluster located in Garching.

year	nodes	main memory (TB)	disk space (TB)
1996	33	0.01	0.5
1998	66	0.06	2.0
2000	95	0.3	8
2002	162	0.6	22
2004	327	2.6	90
2006	345	5.5	190
2008	360	15	510
2010	400	22	560
2012	370	75	770
2014	560	116	1500
2018	600	420	2000
2021	800	1000	4500
2024	1000	1400	6000

3.9.2 Library

The library of the mpi**pks** is a service facility with a wide range of tasks. It is housed in Guest House 4 on three floors ablaze with light. In addition, there is a reading room on the second floor of the main building. This is where international newspapers and copies of the most important books and journals for every group are easily and informally accessible.

Above all, the library provides a large collection of academic books and journals for the use by all members of the mpi**pks** including workshop participants. The library rooms are accessible 24 hours per day and provide scientists with printed media and scientific information in many forms. The automatic check out system permits institute staff to borrow books at any time. A modern Book2net machine and Xerox device enable printing, scanning and copying. Anyone who finds the library atmosphere stimulating for their work or who simply need a desk for their literature search find a quiet desk on the second floor of the library building. Some of these places are reserved for Master's students who are supervised by mpi**pks** group leaders. The library is also open to scientists from outside the institute, but for practical reasons their access is restricted to office hours of the librarian.

Our library collection currently consists of about 5,700 monographs, about 17,300 bound journal volumes and 5 scientific journal subscriptions in print form, which can be easily located via the online catalogue. Readers can use a web form to suggest specific books they need for purchase. This is one way of systematically adding to our book stock. Actually, the number of journal subscriptions in printed form has been drastically reduced in recent years, since most of our researchers now prefer to use electronic access from their own computers. As far as the printed books are concerned, some 120 monographs from the estate of the late founding director Peter Fulde are currently being added to the library's collection.

Our library in guest house 4

Indeed, via the library homepage, mpi**pks** users, identified through the IP address of their computer, have access to about 17,000 peer-reviewed online journals and 900,000 e-books, as well as 200 literature and factual databases, online encyclopedias, dictionaries, MPG Resource Navigator, the e-Doc Server, international catalogues, etc. The discovery system VuFind simplifies the access to various information resources such as the new library online catalogue. All these services also work when connecting to the mpi**pks** computer environment through VPN from home, which was of high relevance during the times of lock-down and home office obligations because of the COVID pandemic. Currently, a major effort is required to migrate the library online catalogue to the open source software Koha which will be finished in fall 2025.

As an additional service, the librarian has access to online document delivery systems. Books or references which are not available in the library or online can be obtained quickly, usually within 24-48 hours, through a simple web-based order form and manual processing by the librarian.

Finally, the library is also responsible for reporting the publication activities of the mpi**pks**, e.g., for the yearbook of the Max Planck Society or the institute's scientific reports. Also the demands of Open Access are related to these activities: The old MPG database e-Doc and the new database PubMan which are institutional repositories with a wide variety of services are fed with the mpi**pks** publications' metadata by the librarian.

The open access policy of the Max Planck Society is fostered by a centralised payment scheme for the article processing charges (APC) for selected journals/publishers, and the information about these is supplied through the library's web-page. For most participating journals this means that if the corresponding author is employed by a Max Planck Institute, then the APCs will be directly covered by the Max Planck Digital Library without involvement of the MPI where the scientist is employed.

A library steering committee of scientists representing the divisions and groups of the mpi**pks** makes sure that the needs of scientists are optimally served by the library. In quarterly meetings decisions such as new journal subscriptions are made.

Our library, as well as most others, is in a transition phase where the classical services continue to be indispensable while new media and new services attain increased relevance. The massive extension of online access to journal articles makes it foreseeable that print issues of journals might be fully replaced by online access in a few years. Most of our online access is organised by the central Max Planck Digital Library MPDL in Munich, who also guarantees the unlimited access to back-issues. In the future, the library will be more and more involved in the dissemination of publications created by the mpi**pks** members through Open Access and an institutional repository.

3.9.3 Guest Houses

To accommodate the large number of short and long term visitors, the Max Planck Institute for the Physics of Complex Systems provides four guest houses with different apartment types for up to 100 guests in total.

Guest houses 1 and 2 © Rene Gaens

Guest house 1 has 20 single and five double rooms (with two separate bedrooms). All of them have a bathroom, a terrace or a balcony, and are equipped with telephones. Our guests use two fully equipped shared kitchens and one meeting room, with a small library and a TV set.

Guest house 2 offers ten one-bedroom apartments with kitchen, and three two-bedroom apartments with living room, bathroom and kitchen for up to three persons (e.g. families). One of the larger apartments is suited for accessible housing. All apartments have a balcony or a terrace, and are equipped with TV connection ports and telephones. In the basement of guest house 2, five washing machines and two tumble dryers are available to all guests.

Guest house 3 allows to accommodate guests in eight large two-bedroom apartments which are well-suited for families with children. On the ground floor, two apartments have been converted into offices in the past, which were used by short term guest scientists or scientists with children. Since additional office space was created in guest house 4 in summer/autumn 2021, the offices in guest house 3 will be re-converted to regular apartments, further increasing the capacities of mpi**pks** to host visitors with families.

The guest houses 1-3 were built in the course of the institute foundation and after 25 years of extensive use they were showing signs of wear. Since their operational readiness is essential for the scientific mission of mpi**pks**, the institute embarked on their renovation. The renovation of both guest houses 1 and 2 was completed by 2024, with the refurbishment of guest house 3 expected to be completed in summer 2025.

Guest house 4 was built in 2012 and offers nine single and two double rooms (with two separate bedrooms). All rooms are equipped with TV connection ports and telephones. Furthermore, the building has a multi-purpose room, which for example is used for German classes, a large terrace and a light garden for the common use and enjoyment. In autumn 2021, it was further improved by the installation of a fully equipped kitchen with a meeting/dining room. Guest house 4 also accommodates six offices for up to 11 scientists, a parent-child office, in case family circumstances require a colleague to bring children to work, the library, and the offices of the visitors program.

The guest house rooms and apartments are cleaned and towels and bed linen are exchanged regularly. Cots can be rented free of charge. WLAN is available in all rooms and apartments.

3.10 Committees

3.10.1 Scientific Advisory Board

According to the rules of the Max Planck Society, the **mpipks** has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and likelihood of success of the research projects, as well as the collaborations among members of the institute, with universities, other research institutions and with industry. The Scientific Advisory Board evaluates the results of the research work presented by the board of directors in the triennial research report and prepares, usually every three years, a report for the President of the Max Planck Society on the research of the institute.
Currently the Scientific Advisory Board has the following members:

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BELGIUM

Singh, R.
Professor Dr.

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3.10.2 Board of Trustees

In accord with the rules of the Max Planck Society the mpi**pks** has formed a Board of Trustees. The board members discuss and consult the proposed budget, the annual report, and the budget of the last year of mpi**pks** together with the directors. The Board of Trustees advises the institute on important issues and promotes the connection of the institute to research oriented circles in the society. The Board of Trustees had the following members during the period of this report (current membership is until December 31, 2030):

Beck, A. Dr.	Ehem. Referatsleiterin Sächsisches Staatsministerium für Wissenschaft, Kultur und Tourismus Wigardstraße 17 01097 Dresden
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Harms, C. Dr.	Kretschmerstraße 21 01309 Dresden
Hilbert, D.	Oberbürgermeister Landeshauptstadt Dresden Dr.-Külz-Ring 19 01067 Dresden
Hollenders, Ch. Dr.	Honorarkonsul Republik Korea Notariat Dr. Hollenders Königstraße 1 01097 Dresden
Kretschmer, M.	Ministerpräsident des Freistaates Sachsen Staatskanzlei Archivstraße 1 01097 Dresden
Milbradt, G. Prof. Dr.	Ministerpräsident des Freistaates Sachsen a.D. Stiller Winkel 4 01328 Dresden
Olbertz, J.-H. Prof. Dr.	Humboldt-Universität zu Berlin Institut für Erziehungswissenschaften Unter den Linden 6 10099 Berlin
Schild, R. Dipl.-Phys.	Am Steinberg 13a 01626 Dresden

Schmidt, F. Dr.-Ing.	Staatssekretär a.D. Birkenstraße 18 01328 Dresden
Pospiech, G. Prof. Dr.	Dekanin der Fachrichtung Physik Technische Universität Dresden 01062 Dresden

3.11 Members of the mpipks

(as of November 2024)

1. mpi**pks positions** — **58**

   - Scientific personnel 17
     Scientific members *3*
     Research staff (including research group leaders) *14*
   - Technical staff 9
   - Administration and infrastructure staff 32

2. **Externally funded research staff** — **8**

3. **PhD students** — **73**

   - PhD students with internal supervision 61
   - PhD students with external supervision 12
     IMPRS PhD students with external supervision *12*
     PhD students with external funding *5*
   - PhD students from Germany 7
   - PhD students from abroad 66

4. **Guest scientists** — **76**

   - Guest scientists from Germany 10
   - Guest scientists from abroad 66

Chapter 4

Publications

4.1 Atomic and Molecular Structure

2021

Gelin, M. F., R. Borrelli, L. Chen: Hierarchical Equations-of-Motion Method for Momentum System-Bath Coupling. The Journal of Physical Chemistry B **125**, 4863-4873 (2021)

Mendez, A. R., L. M. Sandonas, A. Dianat, R. Gutierrez, G. Cuniberti: An Atomistic Study of the Thermoelectric Signatures of CNT Peapods. The Journal of Physical Chemistry C **125**, 13721-13731 (2021)

Ortmann, L., A. AlShafey, A. Staudte, A. S. Landsman: Tracking the Ionization Site in Neutral Molecules. Physical Review Letters **127**, 213201 (2021)

Pal, A., S. Modak, A. Shukla, P. K. Panigrahi: PT-symmetry and supersymmetry: interconnection of broken and unbroken phases. PNAS **477**, 20210494 (2021)

Yan, Y., T. T. Ergogo, Z. Lu, L. Chen, J. Luo, Y. Zhao: Lamb Shift and the Vacuum Rabi Splitting in a Strongly Dissipative Environment. The Journal of Physical Chemistry Letters **12**, 9919-9925 (2021)

Yusipov, I. I., S. V. Denisov, M. Ivanchenko: Chaotic spin-photonic quantum states in an open periodically modulated cavity. Chaos **31**, 013112 (2021)

2022

Ali, E., T. O'Brien, A. Dennis, M. E. Madjet, S. T. Manson, H. S. Chakraborty: Electron vacancy-level dependent hybrid photoionization of the F- @C-60(+) molecule: a novel effect. Journal of Physics B **55**, 045101 (2022)

Johansen, C., J. Lang, A. Morales, A. Baumgartner, T. Donner, F. Piazza: Multimode-polariton superradiance via Floquet engineering. SciPost Physics **12**, 094 (2022)

Rodriguez-Hernandez, F., F. Grossmann, J. M. Rost: Cutoff for continuum-continuum high-order harmonic generation. Physical Review A **105**, L051102 (2022)

Taher-Ghahramani, F., F. Zheng, A. Eisfeld: Gaussian process regression for absorption spectra analysis of molecular dimers. Spectrochimica Acta, Part A **275**, 121091 (2022)

Zhao, Y., K. Sun, L. Chen, M. Gelin: The hierarchy of Davydov's Ansatze and its applications. Wiley Interdisciplinary Reviews: Computational Molecular Science **12**, e1589 (2022)

2023

Bosworth, D. J., F. Hummel, P. Schmelcher: Charged ultralong-range Rydberg trimers. Physical Review A **107**, 022807 (2023)

Hummel, F., P. Schmelcher, M. T. Eiles: Vibronic interactions in trilobite and butterfly Rydberg molecules. Physical Review Research **5**, 013114 (2023)

Li, X.: Estimation of optimal control for two-level and three-level quantum systems with bounded amplitude. Physica Scripta **98**, 105107 (2023)

Matsyshyn, O., J. C. W. Song, I. Sodemann Villadiego, L. Shi: Fermi-Dirac staircase occupation of Floquet bands and current rectification inside the optical gap of metals: An exact approach. Physical Review B **107**, 195135 (2023)

Ruixuan, H., A. Majee, J. Dobnikar, R. Podgornik: Electrostatic interactions between charge regulated spherical macroions. European Physical Journal E **46**, 115 (2023)

Staszewski, L., N. Avidor: Blue shifts in helium-surface bound-state resonances and quantum effects in cosine-law scattering. Physical Chemistry Chemical Physics **25**, 32632-32636 (2023)

2024

Bauer, S., P. Benner, T. Bereau, V. Blum, M. Boley, C. Carbogno, C. R. A. Catlow, G. Dehm, S. Eibl, R. Ernstorfer, A. Fekete, L. Foppa, P. Fratzl, C. Freysoldt, B. Gault, L. M. Ghiringhelli, S. K. Giri, A. Gladyshev, P. Goyal, J. Hattrick-Simpers, L. Kabalan, P. Karpov, M. S. Khorrami, C. T. Koch, S. Kokott, T. Kosch, I. Kowalec, K. Kremer, A. Leitherer, Y. Li, C. H. Liebscher, A. J. Logsdail, Z. Lu, F. Luong, A. Marek, F. Merz, J. R. Mianroodi, J. Neugebauer, Z. Pei, T. A. R. Purcell, D. Raabe, M. Rampp, M. Rossi, J. M. Rost, J. Saal, U. Saalmann, K. N. Sasidhar, A. Saxena, L. Sbailo, M. Scheidgen, M. Schloz, D. F. Schmidt, S. Teshuva, A. Trunschke, Y. Wei, G. Weikum, R. P. Xian, Y. Yao, J. Yin, M. Zhao, M. Scheffler: Roadmap on data-centric materials science. Modelling and Simulation in Materials Science and Engineering **32**, 063301 (2024)

Berngruber, M., D. J. Bosworth, O. A. Herrera-Sancho, V. S. V. Anasuri, N. Zuber, F. Hummel, J. Krauter, F. Meinert, R. Loew, P. Schmelcher, T. Pfau: In Situ Observation of Nonpolar to Strongly Polar Atom-Ion Collision Dynamics. Physical Review Letters **133**, 083001 (2024)

Bosworth, D. J., M. T. Eiles, P. Schmelcher: Metastable doubly charged Rydberg trimers. Physical Review Research **6**, 043164 (2024)

Cioslowski, J., K. Strasburger: Plain Capping for Improved Accuracy of Approximate One- and Two-Electron Densities at Two-Particle Coalescence Points. Journal of Chemical Theory and Computation **20**, 7876-7883 (2024)

Cioslowski, J., K. Strasburger: Constraints upon Functionals of the 1-Matrix, Universal Properties of Natural Orbitals, and the Fallacy of the Collins "Conjecture". The Journal of Physical Chemistry Letters **15**, 1328-1337 (2024)

Eiles, M. T., F. Hummel: Kato's theorem and ultralong-range Rydberg molecules. Physical Review A **109**, 022811 (2024)

4.2 Deterministic Dynamics

2021

Abdou, B., F. I. Ndzana, C. G. L. Tiofack, A. Mohamadou: Stability of one and two-dimensional spatial solitons in a cubic-quintic-septimal nonlinear Schrodinger equation with fourth-order diffraction and PT-symmetric potentials. Wave Motion **107**, 102810 (2021)

Abdou, B., F. Ndzana II, L. G. Tiofack, A. Mohamadou: Linear stability analysis and spatial solitons in the one-dimensional and the two-dimensional generalized nonlinear Schrodinger equation with third-order dispersion and PT-symmetric potentials. European Physical Journal D **75**, 58 (2021)

Akem, N. A., A. M. Dikande, B. Z. Essimbi: Leapfrogging of electrical solitons in coupled nonlinear transmission lines: effect of an imperfect varactor. SN Applied Sciences **2**, 21 (2021)

Ameli, S., M. Karimian, F. Shahbazi: Time-delayed Kuramoto model in the Watts-Strogatz small-world networks. Chaos **31**, 113125 (2021)

An, F. A., K. Padavic, E. J. Meier, S. S. Hegde, S. Ganeshan, J. H. Pixley, S. Vishveshwara, B. Gadway: Interactions and Mobility Edges: Observing the Generalized Aubry-Andre Model. Physical Review Letters **126**, 040603 (2021)

Carney, M., M. Holland, M. Nicol: Extremes and extremal indices for level set observables on hyperbolic systems. Nonlinearity **34**, 1136-1167 (2021)

Diaz-Ruelas, A., F. Baldovin, A. Robledo: Logistic map trajectory distributions: Renormalization-group, entropy, and criticality at the transition to chaos. Chaos **31**, 033112 (2021)

Gallas, J. A. C.: Chirality detected in Hartley's electronic oscillator. The European Physical Journal Plus **136**, 1048 (2021)

Grosvenor, K. T., C. Melby-Thompson, Z. Yan: New heat kernel method in Lifshitz theories. Journal of High Energy Physics 178 (2021)

Hahn, D., J. Urbina, K. Richter, R. Dubertrand, S. L. Sondhi: Ergodic and nonergodic many-body dynamics in strongly nonlinear lattices. Physical Review E **103**, 052213 (2021)

Liu, S., J. Willsher, T. Bilitewski, J. Li, A. Smith, K. Christensen, R. Moessner, J. Knolle: Butterfly effect and spatial structure of information spreading in a chaotic cellular automaton. Physical Review B **103**, 094109 (2021)

Manchein, C., T. M. de Oliveira, R. M. da Silva, M. W. Beims: Collective transient ratchet transport induced by many elastically interacting particles. Scientific Reports **11**, 16178 (2021)

Medjdoub, K., I. M. Jánosi, M. Vincze: Laboratory experiments on the influence of stratification and a bottom sill on seiche damping. Ocean Science **17**, 997-1009 (2021)

Mithun, T., C. Danieli, M. V. Fistul, B. L. Altshuler, S. Flach: Fragile many-body ergodicity from action diffusion. Physical Review E **104**, 014218 (2021)

Negrete Jr., J., I. M. Lengyel, L. Rohde, R. A. Desai, A. C. Oates, F. Jülicher: Theory of time delayed genetic oscillations with external noisy regulation. New Journal of Physics **23**, 033030 (2021)

Rittenhouse, S. T., P. Giannakeas, N. P. Mehta: Scattering of two particles in a one-dimensional lattice. Physical Review A **104**, 023308 (2021)

Sommers, G. M., B. Placke, R. Moessner, S. L. Sondhi: From hard spheres to hard-core spins. Physical Review B **103**, 104407 (2021)

Stoeber, J., A. Bäcker: Geometry of complex instability and escape in four-dimensional symplectic maps. Physical Review E **103**, 042208 (2021)

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Budanur, N. B., H. Kantz: Scale-dependent error growth in Navier-Stokes simulations. Physical Review E **106**, 045102 (2022)

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Gallas, J. A. C., O. Steinbock: Editorial for Focus Issue: From chemical oscillations to applications of nonlinear dynamics: Dedicated to Richard J. Field on the occasion of his 80th birthday. Chaos **32**, 100401 (2022)

Hoyer, C., L. Wetzel, D. Prousalis, J. Wagner, F. Jülicher, F. Ellinger: Mutual Synchronization of Spatially Distributed 24 GHz Oscillators up to Distances of 500 m. IEEE Transactions on Circuits and Systems II **69**, 3689-3693 (2022)

Karpov, P., G. Zhu, M. P. Heller, M. Heyl: Spatiotemporal dynamics of particle collisions in quantum spin chains. Physical Review Research **4**, L032001 (2022)

Kogan, E.: The Kinks, the Solitons and the Shocks in Series-Connected Discrete Josephson Transmission Lines. Physica Status Solidi B **259**, 2200160 (2022)

McRoberts, A. J., T. Bilitewski, M. Haque, R. Moessner: Anomalous dynamics and equilibration in the classical Heisenberg chain. Physical Review B **105**, L100403 (2022)

McRoberts, A. J., T. Bilitewski, M. Haque, R. Moessner: Long-lived solitons and their signatures in the classical Heisenberg chain. Physical Review E **106**, L062202 (2022)

Prousalis, D., L. Wetzel: Synchronization in the presence of time delays and inertia: Stability criteria. Physical Review E **105**, 014210 (2022)

Punetha, N., L. Wetzel: How clock heterogeneity affects synchronization and can enhance stability. Physical Review E **106**, 054216 (2022)

Punetha, N., L. Wetzel: Heterogeneity-induced synchronization in delay-coupled electronic oscillators. Physical Review E **106**, L052201 (2022)

Wetzel, L., D. Prousalis, R. F. Riaz, C. Hoyer, N. Joram, J. Fritzsche, F. Ellinger, F. Jülicher: Network Synchronization Revisited: Time Delays in Mutually Coupled Oscillators. IEEE Access **10**, 80027-80045 (2022)

Yan, J., C. Beck: Information Shift Dynamics Described by Tsallis q=3 Entropy on a Compact Phase Space. Entropy **24**, 1671 (2022)

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Estevez-Moya, D., E. Estevez-Rams, H. Kantz: Complexity and transition to chaos in coupled Adler-type oscillators. Physical Review E **107**, 044212 (2023)

Hoyer, C., L. Wetzel, D. Prousalis, J. Wagner, F. Jülicher, F. Ellinger: Entrainment of Mutually Synchronized Spatially Distributed 24 GHz Oscillators. IEEE transactions on circuits and systems / I **70**, 2665-2678 (2023)

Kogan, E.: Modulated Harmonic Wave in Series-Connected Discrete Josephson Transmission Line: The Discrete Calculus Approach. Physica Status Solidi B **260**, 2200403 (2023)

Kogan, E.: Josephson Transmission Line Revisited. Physica Status Solidi B **260**, 2200475 (2023)

Placke, B., G. M. Sommers, S. L. Sondhi, R. Moessner: Arresting dynamics in hardcore spin models. Physical Review B **107**, L180302 (2023)

Ziebell, L. F., J. A. C. Gallas: Stability of a Duffing oscillator with a position-dependent mass. The European Physical Journal Plus **138**, 930 (2023)

Zimper, S., A. Ngapasare, M. Hillebrand, M. Katsanikas, S. R. Wiggins, C. Skokos: Performance of chaos diagnostics based on Lagrangian descriptors. Application to the 4D standard map. Physical Review D **453**, 133833 (2023)

2024

Adler, D., D. Wei, M. Will, K. Srakaew, S. Agrawal, P. Weckesser, R. Moessner, F. Pollmann, I. Bloch, J. Zeiher: Observation of Hilbert space fragmentation and fractonic excitations in 2D. Nature **636**, 80-85 (2024)

Bednar, H., H. Kantz: Analysis of model error in forecast errors of extended atmospheric Lorenz 05 systems and the ECMWF system. Geoscientific Model Development **17**, 6489-6511 (2024)

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Kurzthaler, C., D. L. Chase, H. A. Stone: Surface corrugations induce helical near-surface flows and transport in microfluidic channels. Journal of Fluid Mechanics **982**, A31 (2024)

McRoberts, A. J., T. Bilitewski, M. Haque, R. Moessner: Domain Wall Dynamics in Classical Spin Chains: Free Propagation, Subdiffusive Spreading, and Soliton Emission. Physical Review Letters **132**, 057202 (2024)

McRoberts, A. J., R. Moessner: Parametrically Long Lifetime of Superdiffusion in Nonintegrable Spin Chains. Physical Review Letters **133**, 256301 (2024)

Moges, H. T., M. Katsanikas, P. A. Patsis, M. Hillebrand, C. Skokos: The Evolution of the Phase Space Structure Along Pitchfork and Period-Doubling Bifurcations in a 3D-Galactic Bar Potential. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering **34**, 2430013 (2024)

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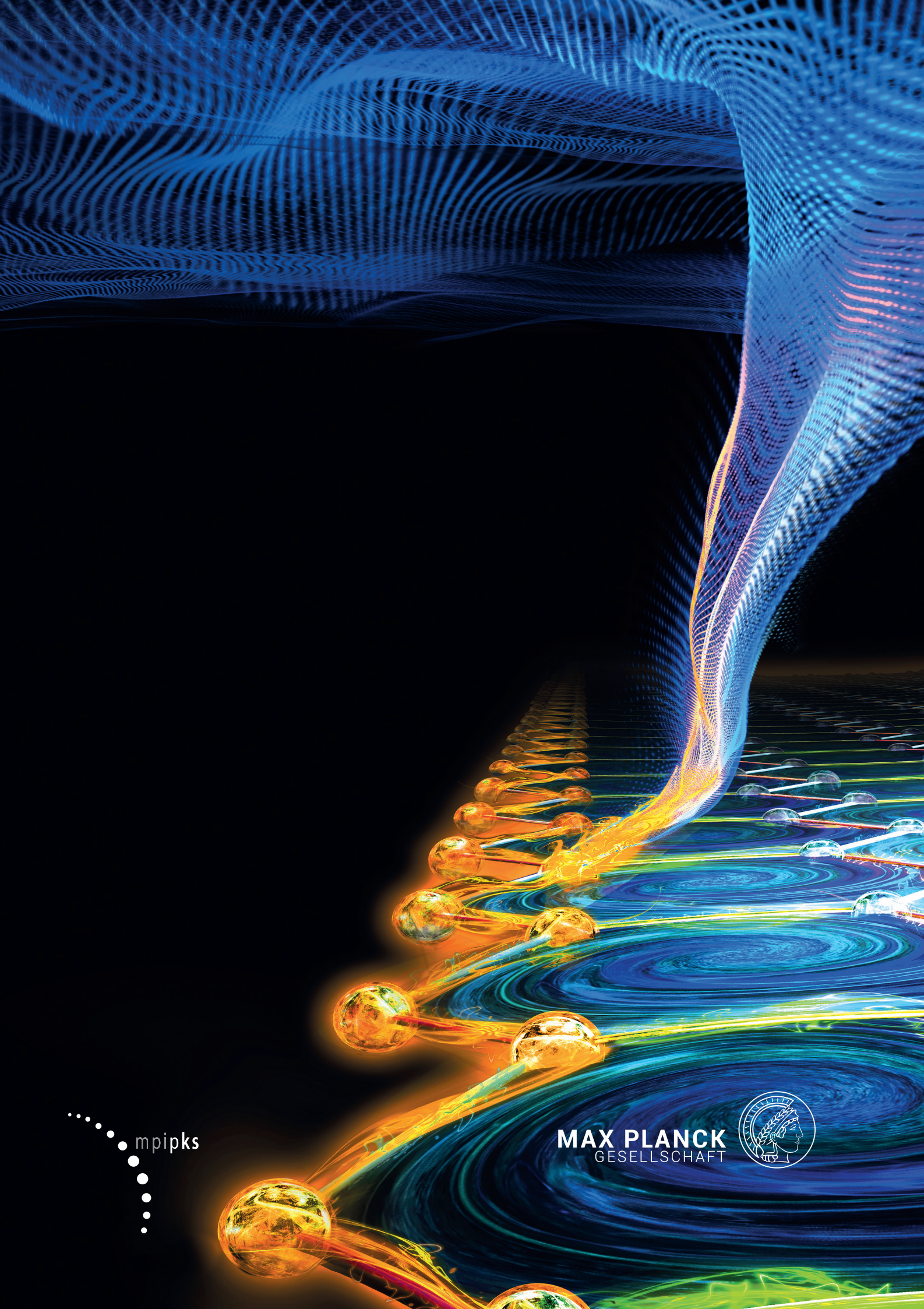
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